

Supporting Information for:

Identification of Potential Solid-State Li-Ion Conductors with Semi-Supervised Learning

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I. Digitized labels for lithium-ion conductors: RT conductivity, activation energy, and corresponding ICSD Identifier

Data labels for the semi-supervised learning approach were ultimately digitized from over 300 literature publications. Many more publications were initially examined. The stepwise decision chart below was used as a guide for deciding what data to digitize. Room temperature conductivity data was only digitized if it originated from an equivalent circuit fit (where a blocking feature was clearly present) or if calculated from NMR. DC techniques were categorically discounted because they cannot differentiate between electronic and ionic conductivity.

Step	Question	Outcome
1	Does the paper have any conductivity data present?	Yes: proceed to step 2. No: find a new paper.
2	Are room-temperature conductivity data values explicitly reported in the text, either from an equivalent circuit fit or NMR?	Yes: record the data. No: proceed to step 3.
3	Are room-temperature conductivity data present in a figure, either from an equivalent circuit fit or NMR?	Yes: digitize the data and record it. No: proceed to step 4.
4	Is the presented data an Arrhenius plot with a linear fit?	Yes: proceed to step 5. No: find a new paper.
5	Digitize the available data. Can a room-temperature conductivity be interpolated from the digitized datapoints?	Yes: record the digitized interpolation. No: proceed to step 6.
6	Does extrapolation of the Arrhenius plot to room temperature result in a value < 1E-10 S cm ⁻¹ ?	Yes: record the data as "<1E-10 S cm ⁻¹ ". No: find a new paper.

All of the digitized data is presented in the subsequent table. Activation energies were also digitized when available. The activation energies were not used in the manuscript but are still presented here to aid future machine learning endeavors. The digitized data was manually matched with the appropriate ICSD ID, so that the crystallographic information file (.cif) can be downloaded. Rows without an associated ICSD ID are highlighted.

Compound	$\sigma_{25^\circ\text{C}}$ (S cm ⁻¹)	E_a (eV)	Space Group	Space Group #	Other names	ICSD	Citation
LiAlSi ₃ O ₈	1.30E-10		C $\bar{1}$	2		81980	¹
LiSn ₂ (PO ₄) ₃	2.04E-9		P $\bar{1}$	2		83832	²
Li ₇ BiO ₆	8.80E-07	0.58	P $\bar{1}$	2		155950	³
Li ₇ SbO ₆	6.70E-08	0.7	P $\bar{1}$	2		413370	³
Li ₇ P ₃ S ₁₁	1.70E-02	0.17	P $\bar{1}$	2		157654	⁴

$\text{Li}_7\text{P}_3\text{S}_{11}$	3.2E-3	0.124	$\text{P}\bar{1}$	2		157654	5
$\text{LiV}(\text{PO}_4)\text{F}$	8.1E-7	0.23	$\text{P}\bar{1}$	2		183876	6
$\text{Li}_2\text{B}_3\text{PO}_8$	5.80E-15	0.76	$\text{P}\bar{1}$	2		248343	7
$\text{Li}_3\text{BP}_2\text{O}_8$	9.60E-12	0.62	$\text{P}\bar{1}$	2		248343	7
$\text{Li}_2\text{NaBP}_2\text{O}_8$	4.40E-18	1.21	$\text{P}\bar{1}$	2		291512	7
$\text{Li}_4\text{P}_2\text{O}_7$	<1E-10	1.617	$\text{P}\bar{1}$	2		248414	8
LiMgSO_4F	5.40E-08	0.54	$\text{P}\bar{1}$	2		281119	9
$\text{Li}_6\text{CuB}_4\text{O}_{10}$	1.00E-13	0.92	$\text{P}\bar{1}$	2	$\beta\text{-Li}_6\text{CuB}_4\text{O}_{10}$	4819	10
$\text{Li}_{0.91}\text{Hf}_{2.022}(\text{PO}_4)_3$	<1E-10	0.47	$\text{C}\bar{1}$	2			11
$\text{Li}_7\text{P}_3\text{S}_{11}$	8.6E-3	0.29	$\text{P}\bar{1}$	2			12
$\text{Li}_2\text{ZnGeO}_4$	1.00E-07	0.4	Pc	7		34362	13
$\text{Li}_{3.8}\text{Ge}_{0.8}\text{P}_{0.2}\text{S}_4$	1.78E-6	0.47	$\text{P}2_1/\text{m}$	11			14
$\text{Li}_{3.6}\text{Ge}_{0.6}\text{P}_{0.4}\text{S}_4$	1.75E-4	0.34	$\text{P}2_1/\text{m}$	11			14
$\text{Li}_{3.4}\text{Ge}_{0.4}\text{P}_{0.6}\text{S}_4$	6.54E-4	0.28	$\text{P}2_1/\text{m}$	11			14
$\text{Li}_{3.35}\text{Ge}_{0.35}\text{P}_{0.65}\text{S}_4$	1.54E-3	0.23	$\text{P}2_1/\text{m}$	11			14
$\text{Li}_{3.3}\text{Ge}_{0.3}\text{P}_{0.7}\text{S}_4$	1.74E-3	0.22	$\text{P}2_1/\text{m}$	11			14
$\text{Li}_{3.25}\text{Ge}_{0.25}\text{P}_{0.75}\text{S}_4$	2.2E-03	0.207	$\text{P}2_1/\text{m}$	11			14
$\text{Li}_{3.2}\text{Ge}_{0.2}\text{P}_{0.8}\text{S}_4$	5.55E-4	0.27	$\text{P}2_1/\text{m}$	11			14
Li_4SiS_4	5.00E-08	0.56	$\text{P}2_1/\text{m}$	11		59708	15
$\text{Li}_{7.22}\text{Si}_{1.5}\text{P}_{0.5}\text{O}_8$	1.64E-7	0.48	$\text{P}2_1/\text{m}$	11		238602	16
Li_4SiO_4	5.00E-10	0.55	$\text{P}2_1/\text{m}$	11		238603	17
Li_4SiS_4	1.59E-8	0.56	$\text{P}2_1/\text{m}$	11			18
$\text{Li}_{3.8}\text{Si}_{0.8}\text{P}_{0.2}\text{S}_4$	8.11E-7	0.37	$\text{P}2_1/\text{m}$	11			18
$\text{Li}_{3.6}\text{Si}_{0.6}\text{P}_{0.4}\text{S}_4$	7.19E-5	0.34	$\text{P}2_1/\text{m}$	11			18

$\text{Li}_{3.5}\text{Si}_{0.5}\text{P}_{0.5}\text{S}_4$	1.66E-4	0.34	P2 ₁ /m	11			18
$\text{Li}_{3.4}\text{Si}_{0.4}\text{P}_{0.6}\text{S}_4$	6.62E-4	0.29	P2 ₁ /m	11			18
$\text{Li}_{3.3}\text{Si}_{0.3}\text{P}_{0.7}\text{S}_4$	1.02E-5	0.36	P2 ₁ /m	11			18
$\text{Li}_{3.2}\text{Si}_{0.2}\text{P}_{0.8}\text{S}_4$	3.20E-6	0.37	P2 ₁ /m	11			18
Li_4SiS_4	1.62E-8	0.56	P2 ₁ /m	11			18
$\text{Li}_{3.8}\text{Si}_{0.8}\text{P}_{0.2}\text{S}_4$	8.07E-7	0.37	P2 ₁ /m	11			18
$\text{Li}_{3.6}\text{Si}_{0.6}\text{P}_{0.4}\text{S}_4$	7.11E-5	0.34	P2 ₁ /m	11			18
$\text{Li}_{3.5}\text{Si}_{0.5}\text{P}_{0.5}\text{S}_4$	1.61E-4	0.34	P2 ₁ /m	11			18
$\text{Li}_{3.4}\text{Si}_{0.4}\text{P}_{0.6}\text{S}_4$	6.49E-4	0.29	P2 ₁ /m	11			18
$\text{Li}_{3.3}\text{Si}_{0.3}\text{P}_{0.7}\text{S}_4$	9.84E-6	0.36	P2 ₁ /m	11			18
$\text{Li}_{3.2}\text{Si}_{0.2}\text{P}_{0.8}\text{S}_4$	3.05E-6	0.37	P2 ₁ /m	11			18
$\text{Li}_{3.1}\text{P}_{0.9}\text{Si}_{0.1}\text{O}_4$	7.47E-8		P21/m	11			19
$\text{Li}_{3.5}\text{P}_{0.5}\text{Si}_{0.5}\text{O}_4$	2.89E-6		P21/m	11			19
$\text{Li}_{3.9}\text{P}_{0.1}\text{Si}_{0.9}\text{O}_4$	1.99E-8		P2 ₁ /m	11			19
$\text{Li}_{3.7}\text{P}_{0.3}\text{Si}_{0.7}\text{O}_4$	3.84E-7		P2 ₁ /m	11		35168	19
Li_3InCl_6	2.04E-3	0.35	C2/m	12		89617	20
$\text{Li}_2\text{P}_2\text{S}_6$	7.80E-11	0.48	C2/m	12		253894	21
$\text{Li}_{0.6}[\text{Li}_{0.2}\text{Sn}_{0.8}\text{S}_2]$	1.2E-4	0.17	C2/m	12			22
$\text{Li}_3(\text{Mo}_8\text{S}_8\text{O}_8(\text{OH})_8(\text{HO}_5(\text{H}_2\text{O}))^*(\text{H}_2\text{O})_{18})$	3.8E-7	0.62	C2/m	12		412011	23
$\text{Li}_{17}\text{Sb}_{13}\text{S}_{28}$	1.05E-9	0.4	C2/m	12		429902	24
Li_3InBr_6	9.04E-4		C2/m	12			25
Li_3YBr_6	1.92E-3	0.37	C2/m	12			26
$\text{Li}_{0.84}\text{Sn}_{0.79}\text{S}_2$	1.2E-4	0.17	C2/m	12			27
$\text{LiAlSi}_4\text{O}_{10}$	1.01E-10		P2/c	13		194284	1
LiPO_3	1.00E-09		P2/c	13		51630	28

LiGaBr ₄	7.00E-6	0.54	P2 ₁ /c	14		61337	25
Li ₂ SO ₄	1.40E-14	1.1	P2 ₁ /c	14		2512	29
Li ₃ BO ₃	7.40E-11	0.63	P2 ₁ /c	14		9105	30
Li ₆ Ge ₂ O ₇	8.50E-07	0.43	P2 ₁ /c	14		31050	31
LiAlCl ₄	1.00E-06	0.47	P2 ₁ /c	14		35275	32
LiYO ₂	1.80E-08	0.72	P2 ₁ /c	14		45511	33
LiBO ₂	1.00E-08	0.71	P2 ₁ /c	14		200891	34
LiClC ₃ H ₇ NO	1.6E-4	0.881	P2 ₁ /c	14		238683	35
LaLiO ₂	<1E-10	0.92	P2 ₁ /c	14		239278	36
(La _{0.9} Sr _{0.1})LiO ₂	6.29E-10	0.62	P2 ₁ /c	14		239279	36
La(Li _{0.76} Mg _{0.08})O ₂	7.27E-10	0.66	P2 ₁ /c	14		239280	36
Li _{2.5} V ₂ (PO ₄) ₃	1.9E-7		P2 ₁ /c	14		240269	37
Li ₄ Zn(PO ₄) ₂	<1E-10	1.3	P2 ₁ /c	14	α -Li ₄ Zn(P O ₄) ₂	255464	38
LiSbO ₂	<1E-10	0.88	P2 ₁ /c	14		262075	39
Li ₂ Sr ₂ Al(PO ₄) ₃	<1E-10	1.02	P2 ₁ /c	14		431319	40
Li ₂ ZrO ₃	6.10E-10	0.78	C2/c	15		94894	33
Li ₆ Zr ₂ O ₇	5.20E-10	0.68	C2/c	15		73835	41
Li ₃ AlF ₆	5.00E-07	0.54	C2/c	15		85171	42
Li ₂ SnS ₃	1.50E-05	0.59	C2/c	15		251656	43
LiTa ₂ PO ₈	1.6E-3	0.32	C2/c	15		267438	44
LiBaP ₂ O ₇	1.00E-10		C2/c	15		280927	45
Li ₃ Na ₅ (TiS ₄) ₂	8.80E-06	0.4	C2/c	15		391258	46
LiGd(PO ₃) ₄	<1E-10	1.7	C2/c	15		416442	47
LiVO ₃	2.048E-9		C2/c	15		51443	48

Li ₂ CrCl ₄	<1E-10	1.22	C2/c	15		202627	49
Li ₃ ErI ₆	9.92E-5	0.37	C2/c	15			50
Li _{3.7} Zn _{0.7} Ga _{0.3} (PO ₄) ₂	<1E-10	0.91	P2 ₁ 2 ₁ 2 ₁	19	β'- Li _{3.7} Zn _{0.7} Ga _{0.3} (P O ₄) ₂	255466	38
Li ₃ SbS ₄	1.5E-6	0.518	Pmn2 ₁	31		8407	51
Li ₃ PS ₄	2.60E-07	0.49	Pmn2 ₁	31	γ-Li ₃ PS ₄	180318	52
LiGaO ₂	2.40E-14	0.86	Pna2 ₁	33		18152	53
LiB ₆ O ₉ F	5.40E-24	1.38	Pna2 ₁	33		420286	54
Li ₃ SbS ₃	1.00E-07	0.4	Pna2 ₁	33		424834	55
LiSi ₂ N ₃	6.17E-08	0.64	Cmc2 ₁	36		34118	56
Li ₂ (PO ₂ N)	<1E-10	0.57	Cmc2 ₁	36		188493	57
LiGa ₂ GeS ₆	3.80E-08	0.47	Fdd2	43		254406	58
La _{0.64} Li _{0.08} TiO ₃	3.35E-4		Pmmm	47		92228	59
La _{0.62} Li _{0.14} TiO ₃	4.42E-4		Pmmm	47		92231	59
La _{0.595} Li _{0.215} TiO ₃	8.53E-4		Pmmm	47		92234	59
Li _{0.4} Na _{0.1} La _{0.5} Nb ₂ O ₆	9.92E-6		Pmmm	47		180629	60
Li _{0.3} Na _{0.2} La _{0.5} Nb ₂ O ₆	1.11E-5		Pmmm	47		180630	60
Li _{0.2} Na _{0.3} La _{0.5} Nb ₂ O ₆	1.18E-5		Pmmm	47		180631	60
Li _{0.1} Na _{0.4} La _{0.5} Nb ₂ O ₆	1.21E-5		Pmmm	47		180632	60
Li _{0.07} Na _{0.43} La _{0.5} Nb ₂ O ₆	1.23E-5		Pmmm	47		180633	60
Li _{0.04} Na _{0.46} La _{0.5} Nb ₂ O ₆	5.91E-6		Pmmm	47		180634	60
Li _{0.02} Na _{0.48} La _{0.5} Nb ₂ O ₆	3.99E-6		Pmmm	47		180635	60
(Ag _{0.33} Li _{0.67}) _{0.27} La _{0.57} TiO ₃	1E-4	0.30	Pmmm	47			61
(Ag _{0.5} Li _{0.5}) _{0.27} La _{0.57} TiO ₃	2.3E-5	0.28	Pmmm	47			61

$(\text{Ag}_{0.67}\text{Li}_{0.33})_{0.27}\text{La}_{0.57}\text{TiO}_3$	2E-7	0.37	Pmmm	47			61
$\text{Pr}_{0.56}\text{Li}_{0.34}\text{TiO}_{3.01}$	1E-6	0.47	Pmmm	47			62
$\text{Nd}_{0.55}\text{Li}_{0.34}\text{TiO}_3$	8E-7	0.53	Pmmm	47			62
$\text{Li}_{0.09}\text{La}_{0.77}\text{TiO}_3$	1.23E-4		Pmmm	47			63
$\text{Li}_{0.15}\text{La}_{0.72}\text{TiO}_3$	4.14E-4		Pmmm	47			63
$\text{Li}_{0.24}\text{La}_{0.65}\text{TiO}_3$	5.77E-4		Pmmm	47			63
$\text{Li}_{0.12}\text{La}_{0.75}\text{TiO}_3$	2.38E-4		Pmmm	47			63
$\text{Li}_{0.16}\text{La}_{0.7}\text{TiO}_3$	5.21E-4		Pmmm	47			63
$\text{Li}_{0.23}\text{La}_{0.7}\text{TiO}_3$	5.26E-4		Pmmm	47			63
Li_5AlO_4	5.00E-10	0.99	Pmmn	59		16229	64
$\text{Li}_{14}\text{Nd}_5(\text{Si}_{11}\text{N}_{19}\text{O}_5)\text{O}_2\text{F}_2$	1.7E-10	0.69	Pmmn	59		262923	65
Li_5GaO_4	5.00E-09	0.71	Pbca	61	$\alpha\text{-Li}_5\text{GaO}_4$	9082	64
Li_2SiN_2	1.60E-07		Pbca	61		420126	66
$\text{Li}_{6.5}\text{O}_8\text{P}_{1.5}\text{Si}_{0.5}$	4.49E-07	0.44	Pnma	62		238600	16
$\text{Li}_{3.4}\text{Si}_{0.7}\text{S}_{0.3}\text{O}_4$	4.21E-7		Pnma	62		47145	67
$\text{Li}_{3.2}\text{Si}_{0.6}\text{S}_{0.4}\text{O}_4$	1.32E-6		Pnma	62			67
$\text{Li}_{3.1}\text{Si}_{0.55}\text{S}_{0.45}\text{O}_4$	3.14E-7		Pnma	62			67
$\text{Li}_{6.6}\text{SiPO}_8$	1.48E-7	0.49	Pnma	62		238601	16
$\text{Li}_{4.2}\text{Si}_{0.8}\text{Al}_{0.2}\text{S}_4$	2.40E-8	0.53	Pnma	62			18
$\text{Li}_{4.4}\text{Si}_{0.6}\text{Al}_{0.4}\text{S}_4$	3.04E-8	0.52	Pnma	62			18
$\text{Li}_{4.6}\text{Si}_{0.4}\text{Al}_{0.6}\text{S}_4$	1.45E-8	0.52	Pnma	62			18
$\text{Li}_{4.8}\text{Si}_{0.2}\text{Al}_{0.8}\text{S}_4$	2.25E-7	0.52	Pnma	62			18
$\text{Li}_{3.8}\text{Si}_{0.8}\text{Al}_{0.2}\text{S}_4$	2.38E-8	0.53	Pnma	62			18
$\text{Li}_{3.6}\text{Si}_{0.6}\text{Al}_{0.4}\text{S}_4$	3.06E-8	0.52	Pnma	62			18

$\text{Li}_{3.4}\text{Si}_{0.4}\text{Al}_{0.6}\text{S}_4$	1.45E-8	0.52	Pnma	62			18
$\text{Li}_{3.2}\text{Si}_{0.2}\text{Al}_{0.8}\text{S}_4$	2.28E-7	0.52	Pnma	62			18
$\text{Li}_4\text{Zn}(\text{PO}_4)_2$	<1E-10	1.1	Pnma	62	$\beta\text{-Li}_4\text{Zn}(\text{PO}_4)_2$	255465	38
$\text{Li}_{3.5}\text{Zn}_{0.5}\text{Ga}_{0.5}(\text{PO}_4)_2$	<1E-10	1.02	Pnma	62	$\beta\text{-Li}_{3.5}\text{Zn}_{0.5}\text{Ga}_{0.5}(\text{PO}_4)_2$	255468	38
Li_3PS_4	1.60E-04	0.36	Pnma	62	$\beta\text{-Li}_3\text{PS}_4$	180319	52
Li_3PO_4	<1E-10	1.14	Pnma	62	$\gamma\text{-Li}_3\text{PO}_4$	20208	68
Li_3PS_4	3.00E-7		Pnma	62	$\gamma\text{-Li}_3\text{PS}_4$	35018	69
$\text{Li}_{2.88}\text{PO}_{3.73}\text{N}_{0.14}$	1.4E-13	0.97	Pnma	62		79426	70
Li_3PO_4	4.2E-18	1.24	Pnma	62	$\gamma\text{-Li}_3\text{PO}_4$	79427	70
Li_4GeS_4	2E-7	0.53	Pnma	62		92200	71
$\text{Li}_{14}\text{Zn}(\text{GeO}_4)_4$	1.00E-06	0.24	Pnma	62		100169	72
$\text{Li}_{3.75}\text{Ge}_{0.75}\text{V}_{0.25}\text{O}_4$	5.66E-6		Pnma	62		150918	73
$\text{Li}_{3.70}\text{Ge}_{0.85}\text{W}_{0.15}\text{O}_4$	3.80E-5		Pnma	62		150920	73
$\text{Li}_{0.2}\text{Ca}_{0.4}\text{TaO}_3$	3.53E-9	0.54	Pnma	62		151936	74
$\text{Li}_{0.2}(\text{Ca}_{0.36}\text{Sr}_{0.04})\text{TaO}_3$	9.2E-9		Pnma	62		151937	74
$\text{Li}_2\text{Mg}_2(\text{MoO}_4)_3$	<1E-10	0.71	Pnma	62		170956	75
Li_4SnSe_4	2E-5	0.45	Pnma	62		193768	76
$\text{Li}(\text{BH}_4)$	1E-8		Pnma	62		239763	77
LiZnSO_4F	2.80E-05	0.2455	Pnma	62		261343	78
Li_4GeS_4	2.00E-07	0.53	Pnma	62		290831	79
Li_4SnS_4	7.0E-5	0.29	Pnma	62		290832	80
Li_2ZnI_4	4.00E-08	0.58	Pnma	62		402062	81

$\text{Pr}_{0.53}\text{Li}_{0.41}\text{TiO}_3$	0.84E-7	0.462	Pnma	62			82
$\text{Pr}_{0.54}\text{Li}_{0.38}\text{TiO}_3$	1.18E-6	0.452	Pnma	62			82
$\text{Pr}_{0.55}\text{Li}_{0.35}\text{TiO}_3$	1.51E-6	0.441	Pnma	62			82
$\text{Pr}_{0.56}\text{Li}_{0.32}\text{TiO}_3$	1.91E-6	0.437	Pnma	62			82
$\text{Pr}_{0.57}\text{Li}_{0.29}\text{TiO}_3$	2.86E-6	0.429	Pnma	62			82
$\text{Pr}_{0.58}\text{Li}_{0.26}\text{TiO}_3$	3.87E-6	0.421	Pnma	62			82
$\text{Pr}_{0.59}\text{Li}_{0.23}\text{TiO}_3$	3.40E-6	0.425	Pnma	62			82
$\text{Li}_{2.5}\text{Y}_{0.5}\text{Zr}_{0.5}\text{Cl}_6$	1.4E-3	0.33	Pnma	62			83
$\text{Li}_{2.633}\text{Er}_{0.633}\text{Zr}_{0.367}\text{Cl}_6$	1.1E-3	0.35	Pnma	62			83
$\text{Li}_{3.33}\text{Ge}_{0.33}\text{V}_{0.67}\text{O}_4$	6.94E-6		Pnma	62			84
$\text{Li}_{3.6}\text{Ge}_{0.6}\text{V}_{0.4}\text{O}_4$	1.97E-5	0.44	Pnma	62			84
$\text{Li}_{3.75}\text{Ge}_{0.75}\text{V}_{0.25}\text{O}_4$	1.08E-5		Pnma	62			84
$\text{Li}_{3.5}\text{Ge}_{0.5}\text{V}_{0.5}\text{O}_4$	1.77E-5		Pnma	62		66576	84
$\text{Li}_{3.87}\text{Sn}_{0.87}\text{As}_{0.13}\text{S}_4$	1.48E-5	0.39	Pnma	62			85
$\text{Li}_{3.855}\text{Sn}_{0.855}\text{As}_{0.145}\text{S}_4$	1.31E-4	0.35	Pnma	62			85
$\text{Li}_{3.85}\text{Sn}_{0.85}\text{As}_{0.15}\text{S}_4$	2.08E-4	0.31	Pnma	62			85
$\text{Li}_{3.84}\text{Sn}_{0.84}\text{As}_{0.16}\text{S}_4$	5.85E-4	0.29	Pnma	62			85
$\text{Li}_{3.83}\text{Sn}_{0.83}\text{As}_{0.17}\text{S}_4$	1.39E-3	0.21	Pnma	62			85
$\text{Li}_{3.825}\text{Sn}_{0.825}\text{As}_{0.175}\text{S}_4$	5.18E-4	0.27	Pnma	62			85
$\text{Li}_{3.82}\text{Sn}_{0.82}\text{As}_{0.18}\text{S}_4$	2.83E-4	0.35	Pnma	62			85
$\text{Li}_{3.8}\text{Sn}_{0.8}\text{As}_{0.2}\text{S}_4$	1.06E-4	0.4	Pnma	62			85
$\text{Li}_{3.75}\text{Sn}_{0.75}\text{As}_{0.25}\text{S}_4$	3.69E-6	0.48	Pnma	62			85
$\text{Nd}_{0.54}\text{Li}_{0.36}\text{TiO}_3$	3.42E-8	0.50	Pnma	62		81047	86
$\text{Pr}_{0.51}\text{Li}_{0.39}\text{TiO}_{2.96}$	5.34E-7	0.44	Pnma	62		81048	86
$\text{Sm}_{0.52}\text{Li}_{0.38}\text{TiO}_{2.97}$	2E-7	0.64	Pnma	62			62

Li ₄ GeO ₄	2.80E-10	0.73	Cmcm	63		18096	87
LiCl*H ₂ O	1E-8	0.777	Cmcm	63		281198	88
Li ₂ MgBr ₄	7.80E-10	0.77	Cmmm	65		73276	89
Li _{0.22} La _{0.60} TiO ₃	4.8E-4	0.391	Cmmm	65			90
Li _{0.18} La _{0.61} TiO ₃	2.0E-4	0.432	Cmmm	65		99398	90
LiBiO ₂	3.80E-08	0.1	Ibam	72		46022	30
Li _{2.5} Zn _{0.25} PS ₄	8.40E-4		I <bar{4}< td=""><td>82</td><td></td><td></td><td>69</td></bar{4}<>	82			69
LiZnPS ₄	5.4E-8		I <bar{4}< td=""><td>82</td><td></td><td>95785</td><td>69</td></bar{4}<>	82		95785	69
Li ₂ Zn _{0.5} PS ₄	1.30E-4	0.22	I <bar{4}< td=""><td>82</td><td></td><td>264462</td><td>69</td></bar{4}<>	82		264462	69
(Li _{1.69} Zn _{0.66})PS ₄	1.30E-4	0.181	I <bar{4}< td=""><td>82</td><td></td><td>264462</td><td>69</td></bar{4}<>	82		264462	69
Li _{1.5} Zn _{0.75} PS ₄	1.65E-5	0.25	I <bar{4}< td=""><td>82</td><td></td><td>264463</td><td>69</td></bar{4}<>	82		264463	69
(Li _{1.19} Zn _{0.9})PS ₄	0.65E-5	0.25	I <bar{4}< td=""><td>82</td><td></td><td>264463</td><td>69</td></bar{4}<>	82		264463	69
(Li _{0.5} Ce _{0.5})(MoO ₄)	1.3E-8	0.4	I4 ₁ /a	88		186450	91
(Li _{0.5} Ce _{0.25} Pr _{0.25})(MoO ₄)	1E-9	0.5	I4 ₁ /a	88		186451	91
(Li _{0.5} Ce _{0.25} Sm _{0.25})(MoO ₄)	1.8E-10	0.5	I4 ₁ /a	88		186452	91
Li ₂ TeO ₄	<1E-10	1.129	P4 ₁ 22	91		1485	92
Li ₃ BN ₂	1.60E-10	0.67	P4 ₂ 12	94	α-Li ₃ BN ₂	655673	93
Li ₂ B ₄ O ₇	1.00E-10		I4 ₁ cd	110		65930	94
LiY(BH ₄) ₄	1.26E-6		P <bar{4}2c< td=""><td>112</td><td></td><td>239762</td><td>77</td></bar{4}2c<>	112		239762	77
LiPN ₂	1.6E-7	0.40	I <bar{4}2d< td=""><td>122</td><td></td><td>66007</td><td>95</td></bar{4}2d<>	122		66007	95
La _{0.565} Li _{0.305} TiO ₃	9.57E-4		P4/mmm	123		92235	59
La _{0.5} Li _{0.5} TiO ₃	9.25E-4	0.39	P4/mmm	123		92236	59
Li _{0.33} La _{0.5} TiO ₃	1E-3	0.15	P4/mmm	123		82671	96
Li _{0.27} La _{0.57} TiO ₃	3.4E-4	0.38	P4/mmm	123			61
La _{0.61} Li _{0.18} TiO ₃	4.12e-4		P4/mmm	123			97

La _{0.55} Li _{0.36} TiO ₃	6.88E-4	0.35	P4/mmm	123			97
La _{0.54} Li _{0.39} TiO ₃	6.51E-4		P4/mmm	123			97
La _{0.52} Li _{0.45} TiO ₃	5.01E-4		P4/mmm	123		50434	97
La _{0.58} Li _{0.27} TiO ₃	5.99E-4		P4/mmm	123		82672	97
La _{0.56} Li _{0.33} TiO ₃	6.68E-4		P4/mmm	123		504435	97
Li _{0.31} La _{0.63} TiO ₃	4.11E-4		P4/mmm	123			63
Li _{0.39} La _{0.59} TiO ₃	8.83E-4		P4/mmm	123			63
Li _{0.49} La _{0.55} TiO ₃	9.39E-4		P4/mmm	123			63
Li _{0.68} La _{0.49} TiO ₃	1.03E-3		P4/mmm	123			63
Li _{0.24} La _{0.65} TiO ₃	9.57E-4		P4/mmm	123			63
Li _{0.33} La _{0.58} TiO ₃	8.93E-4		P4/mmm	123			63
Li _{0.36} La _{0.55} TiO ₃	9.34E-4		P4/mmm	123			63
Li _{0.42} La _{0.52} TiO ₃	8.47E-4		P4/mmm	123			63
Li _{0.29} La _{0.57} TiO ₃	4.4E-5	0.453	P4/mmm	123			90
La _{0.56} Li _{0.33} TiO ₃	1.65E-4	0.41	P4/mmm	123			98
La _{0.56} Li _{0.33} TiO ₃ -5wt% Al ₂ O ₃	1.66E-4	0.24	P4/mmm	123			98
La _{0.56} Li _{0.33} TiO ₃ -10wt% Al ₂ O ₃	9.33E-4	0.17	P4/mmm	123			98
La _{0.56} Li _{0.33} TiO ₃ -15wt% Al ₂ O ₃	9.56E-5	0.50	P4/mmm	123			98
Li(LaTiO ₄)	<1E-10	0.83	P4/nmmZ	129		91843	99
Li(NdTiO ₄)	<1E-10	0.87	P4/nmmZ	129		91844	99
La _{0.65} Li _{0.05} (Mg _{0.5} W _{0.5})O ₃	1.8E-7	0.46	P4/nmm	129		151900	100
La _{0.63} Li _{0.11} (Mg _{0.5} W _{0.5})O ₃	6.8E-6	0.38	P4/nmm	129		151901	100
La _{0.62} Li _{0.14} (Mg _{0.5} W _{0.5})O ₃	1.2E-5	0.37	P4/nmm	129		151902	100

Li ₄ PS ₄ I	1.2E-4	0.37	P4/nmmZ	129		432169	101
Li _{9.75} Sn _{0.75} P _{2.25} S ₁₂	3.57E-3		P4 ₂ /nmcS	137			
Li ₆ ZnO ₄	9.40E-09	0.61	P4 ₂ /nmc	137		62137	64
Li _{9.42} Si _{1.02} P _{2.1} S _{9.96} O _{2.04}	1.1E-4	0.238	P4 ₂ /nmc	137			102
Li _{9.54} Si _{1.74} P _{1.44} S _{11.7} C _{10.3}	2.53E-2	0.238	P4 ₂ /nmc	137			102
Li ₁₀ GeP ₂ S _{11.7} O _{0.3}	1.15E-2	0.155	P4 ₂ /nmc	137			102
Li ₁₀ (Si _{0.5} Sn _{0.5})P ₂ S ₁₂	4.28E-3	0.29	P4 ₂ /nmc	137			102
Li ₉ P ₃ S ₉ O ₃	4.27E-5	0.311	P4 ₂ /nmc	137			103
Li _{10.05} Ge _{1.05} P _{1.95} S ₁₂	1.22E-2	0.28	P4 ₂ /nmc4	137			104
Li _{10.2} Ge _{1.2} P _{1.8} S ₁₂	1.32E-2		P4 ₂ /nmc4	137			104
Li _{10.5} Ge _{1.5} P _{1.5} S ₁₂	1.10E-2		P4 ₂ /nmc 4	137			104
Li ₁₀ GePS ₁₂	1.21E-2		P4 ₂ /nmc	137		188887	104
Li _{10.35} Ge _{1.35} P _{1.65} S ₁₂	1.44E-2	0.269	P4 ₂ /nmc S	137		193947	104
Li _{3.475} Si _{0.475} P _{0.525} S ₄	5.27E-3		P4 ₂ /nmc	137			105
Li _{3.45} Si _{0.45} P _{0.55} S ₄	6.73E-3	0.27	P4 ₂ /nmc	137			105
Li _{3.425} Si _{0.425} P _{0.575} S ₄	5.65E-3		P4 ₂ /nmc	137			105
Li _{3.4} Si _{0.4} P _{0.6} S ₄	4.21E-3		P4 ₂ /nmc	137			105
Li _{3.335} Sn _{0.33} P _{0.67} S ₄	3.73E-3		P4 ₂ /nmc	137			105
Li _{3.3} Sn _{0.3} P _{0.7} S ₄	3.65E-3		P4 ₂ /nmc	137			105
Li _{3.285} Sn _{0.28} P _{0.72} S ₄	4.36E-3		P4 ₂ /nmc	137			105
Li _{3.27} Sn _{0.27} P _{0.73} S ₄	4.96E-3		P4 ₂ /nmc	137			105
Li _{3.26} Sn _{0.26} P _{0.74} S ₄	4.53E-3		P4 ₂ /nmc	137			105
Li _{3.25} Sn _{0.25} P _{0.75} S ₄	3.6E-3		P4 ₂ /nmc	137			105
Li ₁₀ SiP ₂ S ₁₂	2.3E-3	0.196	P42/nmc	137			106
Li ₁₀ SnP ₂ S ₁₂	7E-3	0.27	P4 ₂ /nmc C	137		193755	107

$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	2.46E-2	0.274	P4 ₂ /nmc	137		241439	108
$\text{Li}_{10}(\text{Ge}_{0.776}\text{Sn}_{0.224})\text{P}_2\text{S}_{12}$	1.41E-2	0.276	P4 ₂ /nmc	137		255748	108
$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	3.98E-3	0.305	P4 ₂ /nmc	137		255750	108
$\text{Li}_{10}(\text{Ge}_{0.416}\text{Sn}_{0.584})\text{P}_2\text{S}_{12}$	7.43E-3	0.285	P4 ₂ /nmc	137		255757	108
$\text{Li}_{10.35}\text{Si}_{1.35}\text{P}_{1.65}\text{S}_{12}$	6.5E-3		P4 ₂ /nmcS	137		252037	109
$\text{Li}_{9.81}\text{Sn}_{0.81}\text{P}_{2.19}\text{S}_{12}$	5.5E-3		P4 ₂ /nmc	137		252040	109
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	1.20E-02	0.25	P4 ₂ /nmc	137		255749	110
$\text{Li}_{10.2}\text{Si}_{1.2}\text{P}_{1.8}\text{S}_{12}$	4.16E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{10.275}\text{Si}_{1.275}\text{P}_{1.725}\text{S}_{12}$	5.61E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{10.35}\text{Si}_{1.35}\text{P}_{1.65}\text{S}_{12}$	6.68E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{10.425}\text{Si}_{1.425}\text{P}_{1.575}\text{S}_{12}$	5.22E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	1.21E-2		P4 ₂ /nmcS	137			111
$\text{Li}_{10.05}\text{Ge}_{1.05}\text{P}_{1.95}\text{S}_{12}$	1.25E-2		P4 ₂ /nmcS	137			111
$\text{Li}_{10.2}\text{Ge}_{1.2}\text{P}_{1.8}\text{S}_{12}$	1.36E-2		P4 ₂ /nmcS	137			111
$\text{Li}_{10.35}\text{Ge}_{1.35}\text{P}_{1.65}\text{S}_{12}$	1.41E-2		P4 ₂ /nmcS	137			111
$\text{Li}_{10.5}\text{Ge}_{1.5}\text{P}_{1.5}\text{S}_{12}$	1.09E-2		P4 ₂ /nmcS	137			111
$\text{Li}_{9.79}\text{Sn}_{0.79}\text{P}_{2.21}\text{S}_{12}$	4.56E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{9.81}\text{Sn}_{0.81}\text{P}_{2.19}\text{S}_{12}$	4.98E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{9.87}\text{Sn}_{0.87}\text{P}_{2.13}\text{S}_{12}$	4.32E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{9.9}\text{Sn}_{0.9}\text{P}_{2.1}\text{S}_{12}$	3.66E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	3.65E-3		P4 ₂ /nmcS	137			111
$\text{Li}_{10.2}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.2}\text{P}_{1.8}\text{S}_{12}$	7.82E-3		P4 ₂ /nmcS	137		5667	111
$\text{Li}_{10.5}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.5}\text{P}_{1.5}\text{S}_{12}$	8.79E-3		P4 ₂ /nmcS	137		5668	111
$\text{Li}_{10.35}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.35}\text{P}_{1.65}\text{S}_{12}$	1.08E-2		P4 ₂ /nmcS	137		5669	111

$\text{Li}_{10.35}(\text{Sn}_{0.27}\text{Si}_{1.08})\text{P}_{1.65}\text{S}_{12}$	1.1E-3	0.197	P4 ₂ /nmcS	137		257946	111
$\text{Li}_{10.2}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.2}\text{P}_{1.8}\text{S}_{12}$	2.69E-3		P4 ₂ /nmcS	137		257948	111
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	1.43E-3	0.24	P4 ₂ /nmcS	137			112
$\text{Li}_{9.8}\text{Ba}_{0.1}\text{GeP}_2\text{S}_{12}$	5.61E-4		P4 ₂ /nmcS	137			112
$\text{Li}_{9.6}\text{Ba}_{0.2}\text{GeP}_2\text{S}_{12}$	5.72E-4		P4 ₂ /nmcS	137			112
$\text{Li}_{9.4}\text{Ba}_{0.3}\text{GeP}_2\text{S}_{12}$	7.07E-4	0.29	P4 ₂ /nmcS	137			112
$\text{Li}_{9.2}\text{Ba}_{0.4}\text{GeP}_2\text{S}_{12}$	3.16E-4		P4 ₂ /nmcS	137			112
$\text{Li}_9\text{Ba}_{0.5}\text{GeP}_2\text{S}_{12}$	9.98E-5		P4 ₂ /nmcS	137			112
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	5.0E-3	0.35	P4 ₂ /nmc	137			113
$\text{LiLaNb}_2\text{O}_7$	<1E-8		I4/mmm	139		72566	114
$\text{Li}_4\text{Sr}_3\text{Nb}_{5.77}\text{Fe}_{0.23}\text{O}_{19.77}$	<1E-10		I4/mmm	139		87823	115
$\text{Li}_4\text{Sr}_3\text{Nb}_6\text{O}_{20}$	<1E-10		I4/mmm	139		87824	115
$\text{Li}_4\text{Sr}_{3.056}\text{Nb}_6\text{O}_{20}$	<1E-10	0.74	I4/mmm	139		109168	115
LiScO_2	1.00E-12	0.87	I4 ₁ /amd	141		36124	33
r-LiAlO ₂	1.10E-12	0.97	I4 ₁ /amd	141		99517	33
Li_3BN_2	8.70E-08	0.55	I4 ₁ /amd	141	$\beta\text{-Li}_3\text{BN}_2$	155126	93
Li_4SrN_2	2.30E-13	0.9	I4 ₁ /amd	141		87413	116
LiScO_2	<1E-10	1.047	I4 ₁ /amd	141		257819	117
$\text{Li}_{0.9}\text{Sc}_{0.9}\text{Zr}_{0.1}\text{O}_2$	<1E-10	0.912	I4 ₁ /amd	141		257820	117
$\text{Li}_7\text{La}_3\text{HfO}_{12}$	9.85E-7	0.53	I4 ₁ /acdZ	142	“tetragonal-LLHO”	174202	118
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.63E-6	0.54	I4 ₁ /acdZ	142	“tetragonal-LLZO”	183684	119
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	5E-7	0.59	I4 ₁ /acdZ	142			120
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	9.9E-6	0.43	I4 ₁ /acdZ	142		238687	121

LiGaSiO ₄	3.00E-16	0.9	R3H	146		65125	122
LiGa _{0.5} Al _{0.5} GeO ₄	<1E-10	1.06	R3H	146		257740	123
LiAlGeO ₄	<1E-10	0.97	R3H	146		257741	123
LiGaGeO ₄	<1E-10	1.12	R̄3	148		257739	123
LiTi ₂ (PO ₄) ₃	1.61E-4	0.21	R̄3	148			124
Li _{1.2} Ti _{1.8} Al _{0.2} (PO ₄) ₃	4.82E-3	0.18	R̄3	148			124
LiNaSO ₄	8.80E-10		P31c	159		14364	125
Li _{3.333} Mg _{0.333} P ₂ S ₆	8.20E-8	0.517	P̄31m	162		95606	126
Li _{2.667} Mg _{0.667} P ₂ S ₆	4.00E-06	0.46	P̄31m	162		95607	126
Li ₄ P ₂ S ₆	2.38E-07	0.29	P̄31m	162		242170	127
Li ₄ P ₂ S ₆	1.6E-10	0.48	P̄31m	162			128
Li ₃ YCl ₆	5.39E-4	0.40	P̄3m1	164			26
Li ₃ ErCl ₆	3.3E-4	0.41	P̄3m1	164		50151	129
Li _{4.4} Al _{0.4} Ge _{0.6} S ₄	4.33E-5	0.38	P̄3m1	164		235201	130
Li _{4.4} Al _{0.4} Sn _{0.6} S ₄	3.6E-6	0.15	P̄3m1	164		235207	130
Li ₅ NCl ₂	1.20E-06	0.5	R̄3m	166		84763	131
LiHf ₂ (PO ₄) ₃	2.833E-7		R̄3cH	167			2
LiZr ₂ (PO ₄) ₃	2.96E-10		R̄3cH	167		201935	2
LiGe ₂ (PO ₄) ₃	3.33E-7		R̄3cH	167		263767	2
Li _{1.1} Ti _{1.9} Sc _{0.1} (PO ₄) ₃	3.89E-4	0.3	R̄3cH	167			132
Li _{1.2} Ti _{1.8} Sc _{0.2} (PO ₄) ₃	2.51E-3	0.25	R̄3cH	167			132
Li _{1.3} Ti _{1.7} Sc _{0.3} (PO ₄) ₃	7.91E-4	0.28	R̄3cH	167			132
Li _{1.4} Ti _{1.6} Sc _{0.4} (PO ₄) ₃	1.99E-4	0.31	R̄3cH	167			132
Li _{1.5} Ti _{1.5} Sc _{0.5} (PO ₄) ₃	9.74E-5	0.32	R̄3cH	167			132
LiTi ₂ (PO ₄) ₃	7.61E-6	0.38	R̄3cH	167		95979	132

$\text{LiGe}_2(\text{PO}_4)_3$	4.83E-9	0.654	R $\bar{3}$ cH	167		69763	133
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Ge}_{1.8}(\text{PO}_4)_3$	4.83E-5	0.387	R $\bar{3}$ cH	167		263760	133
$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ge}_{1.6}(\text{PO}_4)_3$	1.88E-4	0.407	R $\bar{3}$ cH	167		263762	133
$\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	3.36E-4	0.426	R $\bar{3}$ cH	167		263763	133
$\text{Li}_{1.7}\text{Al}_{0.7}\text{Ge}_{1.3}(\text{PO}_4)_3$	2.64E-4	0.450	R $\bar{3}$ cH	167		263765	133
$\text{Li}_{1.8}\text{Al}_{0.8}\text{Ge}_{1.2}(\text{PO}_4)_3$	1.37E-4	0.429	R $\bar{3}$ cH	167		263766	133
$\text{LiTi}_2(\text{PO}_4)_3$	1.0E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{Ti}_2\text{Si}_{0.2}\text{P}_{2.8}\text{O}_{12}$	8.6E-5		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{Ti}_2\text{Si}_{0.3}\text{P}_{2.7}\text{O}_{12}$	3.2E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{Ti}_2\text{Si}_{0.4}\text{P}_{2.6}\text{O}_{12}$	1.5E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{Ti}_2\text{Si}_{0.5}\text{P}_{2.5}\text{O}_{12}$	9.6E-5		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	3E-3		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	3.88E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{Al}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	2.48E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{Cr}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	1.82E-5		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{Cr}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	3.51E-5		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{Cr}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	1.49E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{Cr}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	3.86E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.6}\text{Cr}_{0.6}\text{Ti}_{1.4}(\text{PO}_4)_3$	1.26E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.7}\text{Cr}_{0.7}\text{Ti}_{1.3}(\text{PO}_4)_3$	8.05E-6		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{Ga}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	1.62E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{Ga}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	2.61E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{Ga}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	1.28E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{Ga}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	1.22E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{Fe}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	1.80E-4		R $\bar{3}$ cH	167			134

$\text{Li}_{1.3}\text{Fe}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	2.46E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{Fe}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	3.92E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{Sc}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	6.90E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{Sc}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	7.03E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{Sc}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	5.15E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{Sc}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	2.53E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{In}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	3.90E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{In}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	3.93E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{In}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	3.02E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{In}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	2.04E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.2}\text{La}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	8.00E-5		R $\bar{3}$ cH	167			134
$\text{Li}_{1.3}\text{La}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	5.23E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.4}\text{La}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	4.98E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{La}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	2.81E-4		R $\bar{3}$ cH	167			134
$\text{Li}_{1.5}\text{Fe}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	1.74E-4		R $\bar{3}$ cH	167		55751	134
$\text{Li}_{0.87}\text{Hf}_{2.032}\text{P}_3\text{O}_{12}$	1.29E-05	0.33	R $\bar{3}$ cH	167		83501	134
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	5.95E-4		R $\bar{3}$ cH	167		427621	134
$\text{Li}(\text{Ti}_{1.4}\text{Sn}_{0.6})(\text{PO}_4)_3$	2.28E-5	0.32	R $\bar{3}$ cH	167		183672	135
$\text{Li}(\text{Ti}_{0.6}\text{Sn}_{1.4})(\text{PO}_4)_3$	9.42E-6		R $\bar{3}$ cH	167		183676	135
$\text{Li}(\text{Ti}_{0.4}\text{Sn}_{1.6})(\text{PO}_4)_3$	3.15E-6		R $\bar{3}$ cH	167		183677	135
$\text{Li}_{1.15}\text{Y}_{0.15}\text{Zr}_{1.85}(\text{PO}_4)_3$	1.4E-4	0.39	R $\bar{3}$ cH	167		191891	136
$\text{LiZr}_2(\text{PO}_4)_3$	1E-9	0.76	R $\bar{3}$ cH	167		201935	137
$\text{Li}_{1.3}(\text{Al}_{0.3}\text{Ti}_{1.7})(\text{PO}_4)_3$	8.02E-7		R $\bar{3}$ cH	167		253240	138
$\text{Li}_{1.3}(\text{Al}_{0.23}\text{Ga}_{0.07}\text{Ti}_{1.7})(\text{PO}_4)_3$	4.46E-6		R $\bar{3}$ cH	167		253241	138

$\text{Li}_{1.3}(\text{Al}_{0.23}\text{Sc}_{0.07}\text{Ti}_{1.7})(\text{PO}_4)_3$	1.94E-7		R $\bar{3}$ cH	167		253242	138
$\text{Li}_{1.3}(\text{Al}_{0.23}\text{Y}_{0.07}\text{Ti}_{1.7})(\text{PO}_4)_3$	3.84E-8		R $\bar{3}$ cH	167		253243	138
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	7E-4		R $\bar{3}$ cH	167		257190	139
$\text{LiZr}_2(\text{PO}_4)_3$	8.5E-5		R $\bar{3}$ cH	167			140
$\text{Li}_{1.025}\text{Y}_{0.025}\text{Zr}_{1.975}(\text{PO}_4)_3$	1.28E-4		R $\bar{3}$ cH	167			140
$\text{Li}_{1.05}\text{Y}_{0.05}\text{Zr}_{1.95}(\text{PO}_4)_3$	1.3E-4		R $\bar{3}$ cH	167			140
$\text{Li}_{1.1}\text{Y}_{0.1}\text{Zr}_{1.9}(\text{PO}_4)_3$	1.0E-4		R $\bar{3}$ cH	167			140
$\text{Li}_{1.1}\text{Al}_{0.1}\text{Ge}_{1.9}(\text{PO}_4)_3$	1.29E-5		R $\bar{3}$ cH	167			140
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Ge}_{1.8}(\text{PO}_4)_3$	1.89E-5	0.46	R $\bar{3}$ cH	167			140
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	1.91E-4		R $\bar{3}$ cH	167			140
$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ge}_{1.6}(\text{PO}_4)_3$	3.17E-4	0.37	R $\bar{3}$ cH	167			140
$\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	3.45E-4		R $\bar{3}$ cH	167			140
$\text{Li}_{1.6}\text{Al}_{0.6}\text{Ge}_{1.4}(\text{PO}_4)_3$	3.94E-4	0.37	R $\bar{3}$ cH	167			140
$\text{Li}_{1.7}\text{Al}_{0.7}\text{Ge}_{1.3}(\text{PO}_4)_3$	2.75E-4		R $\bar{3}$ cH	167			140
$\text{Li}_{1.8}\text{Al}_{0.8}\text{Ge}_{1.2}(\text{PO}_4)_3$	1.23E-4	0.43	R $\bar{3}$ cH	167			140
$\text{LiGe}_2(\text{PO}_4)_3$	3.12E-9	0.60	R $\bar{3}$ cH	167			141
$\text{Li}_{0.86}\text{Hf}_{2.035}(\text{PO}_4)_3$	9.2E-8	0.48	R $\bar{3}$ cH	167			11
$\text{Li}_{1.7}\text{Al}_{0.3}\text{Ti}_{1.6}(\text{PO}_4)_3$	5E-5		R $\bar{3}$ cH	167			142
$\text{Li}_{1.2}\text{In}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	8.22E-5	0.32	R $\bar{3}$ cH	167			143
$\text{Li}_{1.3}\text{Al}_{0.2}\text{Sc}_{0.1}\text{Ti}_{1.7}(\text{PO}_4)_3$	9.72E-4	0.25	R $\bar{3}$ cH	167			144
$\text{Li}_{1.3}\text{Al}_{0.15}\text{Sc}_{0.15}\text{Ti}_{1.7}(\text{PO}_4)_3$	1.24E-3	0.23	R $\bar{3}$ cH	167			144
$\text{Li}_{1.3}\text{Al}_{0.1}\text{Sc}_{0.2}\text{Ti}_{1.7}(\text{PO}_4)_3$	4.29E-4	0.26	R $\bar{3}$ cH	167			144
$\text{Li}_{1.3}\text{Sc}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	4.52E-4	0.25	R $\bar{3}$ cH	167			144

$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	1.13E-3	0.23	R $\bar{3}$ cH	167		257190	144
$\text{LiTi}(\text{PO}_4)_3$	6E-5	0.33	R $\bar{3}$ c	167			145
$\text{Li}_{1.05}\text{Al}_{0.05}\text{Ti}_{0.95}(\text{PO}_4)_3$	1.1E-3	0.31	R $\bar{3}$ c	167			145
$\text{Li}_{1.1}\text{Al}_{0.1}\text{Ti}_{0.9}(\text{PO}_4)_3$	6.7E-4	0.32	R $\bar{3}$ c	167			145
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Ti}_{0.8}(\text{PO}_4)_3$	4.0E-3	0.31	R $\bar{3}$ c	167			145
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{0.7}(\text{PO}_4)_3$	6.2E-3	0.30	R $\bar{3}$ c	167			145
$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}_{0.6}(\text{PO}_4)_3$	3.3E-3	0.29	R $\bar{3}$ c	167			145
$\text{Li}_{1.05}\text{Cr}_{0.05}\text{Ti}_{0.95}(\text{PO}_4)_3$	1.8E-4	0.33	R $\bar{3}$ c	167			145
$\text{Li}_{1.1}\text{Cr}_{0.1}\text{Ti}_{0.9}(\text{PO}_4)_3$	2.6E-4	0.32	R $\bar{3}$ c	167			145
$\text{Li}_{1.2}\text{Cr}_{0.2}\text{Ti}_{0.8}(\text{PO}_4)_3$	4.3E-4	0.31	R $\bar{3}$ c	167			145
$\text{Li}_{1.3}\text{Cr}_{0.3}\text{Ti}_{0.7}(\text{PO}_4)_3$	2.9E-4	0.32	R $\bar{3}$ c	167			145
$\text{Li}_{1.05}\text{Fe}_{0.05}\text{Ti}_{0.95}(\text{PO}_4)_3$	1.3E-4	0.34	R $\bar{3}$ c	167			145
$\text{Li}_{1.1}\text{Fe}_{0.1}\text{Ti}_{0.9}(\text{PO}_4)_3$	6.3E-4	0.34	R $\bar{3}$ c	167			145
$\text{Li}_{1.2}\text{Fe}_{0.2}\text{Ti}_{0.8}(\text{PO}_4)_3$	1.4E-3	0.32	R $\bar{3}$ c	167			145
$\text{Li}_{1.3}\text{Fe}_{0.3}\text{Ti}_{0.7}(\text{PO}_4)_3$	2.3E-3	0.31	R $\bar{3}$ c	167			145
$\text{Li}_{1.5}\text{Fe}_{0.5}\text{Ti}_{0.5}(\text{PO}_4)_3$	2.7E-4	0.32	R $\bar{3}$ c	167			145
$\text{LiGe}_2(\text{PO}_4)_3$	3.37E-7	0.38	R $\bar{3}$ c	167			146
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	1.42E-4	0.37	R $\bar{3}$ c	167			146
$\text{Li}_{1.7}\text{Al}_{0.7}\text{Ge}_{1.3}(\text{PO}_4)_3$	2.04E-4		R $\bar{3}$ c	167			146
$\text{Li}_{1.3}\text{Cr}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	8.87E-5	0.39	R $\bar{3}$ c	167			146
$\text{Li}_{1.5}\text{Cr}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	1.21E-4	0.37	R $\bar{3}$ c	167			146
$\text{Li}_{1.7}\text{Cr}_{0.7}\text{Ge}_{1.3}(\text{PO}_4)_3$	2.46E-5		R $\bar{3}$ c	167			146
$\text{Li}_{1.3}\text{Ga}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	4.47E-5	0.38	R $\bar{3}$ c	167			146
$\text{Li}_{1.5}\text{Ga}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	2.01E-5		R $\bar{3}$ c	167			146
$\text{Li}_{1.3}\text{Fe}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	2.99E-5	0.39	R $\bar{3}$ c	167			146

$\text{Li}_{1.5}\text{Fe}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	2.56E-5		R $\bar{3}$ c	167			146
$\text{Li}_{1.3}\text{Sc}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	5.59E-5		R $\bar{3}$ c	167			146
$\text{Li}_{1.3}\text{In}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	9.22E-6		R $\bar{3}$ c	167			146
$\text{Li}_{1.5}\text{In}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	5.81E-6		R $\bar{3}$ c	167			146
$\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$	2.86E-4	0.38	R $\bar{3}$ c	167		263764	146
LiIO_3	1.90E-07		P6 ₃	173		35473	147
$\text{Li}_9\text{Mg}_3(\text{PO}_4)_4\text{F}_3$	<1E-10	0.835	P6 ₃	173		426103	148
$\text{Pb}_{6.12}\text{Ca}_{1.9}\text{Li}_{1.96}(\text{PO}_4)_6$	<1E-10	1.05	P6/m	176		59615	149
LiNdSiO_4	<1E-10		P6/m	176			150
LiDySiO_4	<1E-10		P6/m	176			150
$\text{Li}_2\text{La}_8\text{Si}_6\text{O}_{25}$	<1E-10		P6/m	176			150
$\text{Li}_3\text{La}_7\text{Si}_6\text{O}_{24}$	<1E-10		P6/m	176			150
$\text{Li}_{0.284}\text{Sm}_{4.512}\text{Si}_3\text{O}_{12.91}$	<1E-10		P6/m	176		83279	150
$\text{LiLa}_9\text{Si}_6\text{O}_{26}$	<1E-10		P6/m	176		291218	150
$\text{LiEu}_9\text{Si}_6\text{O}_{26}$	<1E-10		P6/m	176		291220	150
LiAlSiO_4	2.00E-09	0.68	P6 ₄ 22	181		55665	151
$\text{Li}_3(\text{NH}_2)_2\text{I}$	1E-5	0.58	P6 ₃ mc	186		167528	152
$\text{Ba}_3\text{LiTa}_5\text{ZrSi}_4\text{O}_{26}$	<1E-10	0.79	P6 ₂ m	189		239277	153
Li_3N	1.2E-3	0.25	P6/mmm	191		26540	154
Li_3N	3.00E-04	0.26	P6/mmm	191		156894	155
$\text{Fe}_2\text{Na}_2\text{K}(\text{Li}_3\text{Si}_{12}\text{O}_{30})$	<1E-10	1.22	P6/mcc	192		235750	156
Li_3P	7.03E-4	0.18	P6 ₃ /mmc	194		642223	157
$\text{Li}_{5.5}\text{K}_{0.25}\text{La}_{2.75}\text{Nb}_2\text{O}_{12}$	3.19E-3	0.49	I2 ₁ 3	199			158
$\text{Li}_{5.5}\text{La}_3\text{Nb}_{1.75}\text{In}_{0.25}\text{O}_{12}$	8.07E-3	0.49	I2 ₁ 3	199			158
$\text{Li}_6\text{BaLa}_2\text{Nb}_2\text{O}_{12}$	6E-6	0.44	I2 ₁ 3	199			159

$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	8E-6	0.43	I2 ₁ 3	199		54865	159
(K _{0.1} Li _{0.9})(SbO ₃)	1.36E-8		Pn $\bar{3}$ Z	201		200984	160
Li_8GeP_4	1.8E-5	0.435	Pa $\bar{3}$	205	α - Li_8GeP_4	235184	161
Li_8SiP_4	4.5E-5	0.404	Pa $\bar{3}$	205		235186	161
Li_3AlN_2	5.00E-08	0.45	Ia $\bar{3}$	206		257464	162
$\text{Li}_2\text{MgTi}_3\text{O}_8$	<1E-10	0.71	P4 ₃ 2	212		86165	163
$\text{Li}_2\text{CoTi}_3\text{O}_8$	<1E-10	1.33	P4 ₃ 2	212		86166	163
$\text{Li}_2\text{CoGe}_3\text{O}_8$	<1E-10	1.49	P4 ₃ 2	212		86167	163
$\text{Li}_2\text{ZnGe}_3\text{O}_8$	<1E-10	2.14	P4 ₃ 2	212		86169	163
(Li _{0.61} Mg _{0.39})(Li _{0.46} Mg _{0.00} 5Ti _{0.035})Ti _{1.5} O ₄	6.56E-10	0.685	P4 ₃ 2	212		168144	164
(Li _{0.55} Mg _{0.45})(Li _{0.445} Mg _{0.0} 55)Ti _{1.5} O ₄	1.53E-11	0.786	P4 ₃ 2	212		168145	164
Li_5NiI_2	4.00E-6		F $\bar{4}3m$	216		16800	165
Li_2VCl_4	6.95E-6		F $\bar{4}3m$	216		74959	166
$\text{Li}_6\text{PS}_5\text{Cl}_{0.25}\text{Br}_{0.75}$	1.86E-3	0.328	F $\bar{4}3m$	216			167
$\text{Li}_6\text{PS}_5\text{Cl}$	2.05E-3	0.452	F $\bar{4}3m$	216		259200	167
$\text{Li}_6\text{PS}_5\text{Cl}_{0.5}\text{Br}_{0.5}$	3.33E-3	0.367	F $\bar{4}3m$	216		259201	167
$\text{Li}_6\text{PS}_5\text{Br}$	1.15E-3	0.303	F $\bar{4}3m$	216		259202	167
$\text{Li}_6\text{PS}_5\text{Br}_{0.5}\text{I}_{0.5}$	2.62E-5	0.312	F $\bar{4}3m$	216		259203	167
$\text{Li}_6\text{PS}_5\text{I}$	1.3E-6	0.383	F $\bar{4}3m$	216		259204	167
$\text{Li}_6\text{PS}_5\text{Cl}_{0.75}\text{Br}_{0.25}$	2.26E-3	0.408	F $\bar{4}3m$	216		259206	167
$\text{Li}_6\text{PS}_5\text{Br}_{0.75}\text{I}_{0.25}$	1.12E-4	0.321	F $\bar{4}3m$	216		259209	167
$\text{Li}_6\text{PS}_5\text{Br}_{0.25}\text{I}_{0.75}$	4.72E-6	0.351	F $\bar{4}3m$	216		259211	167
$\text{Li}_6\text{PS}_5\text{Br}$	7.01E-4	0.194	F $\bar{4}3m$	216		234584	168

$\text{Li}_{6.025}\text{P}_{0.975}\text{Si}_{0.025}\text{S}_5\text{Br}$	8.78E-4	0.196	$\bar{\text{F}43m}$	216		234585	168
$\text{Li}_{6.05}\text{P}_{0.95}\text{Si}_{0.05}\text{S}_5\text{Br}$	4.37E-4	0.173	$\bar{\text{F}43m}$	216		234586	168
$\text{Li}_{6.075}\text{P}_{0.925}\text{Si}_{0.075}\text{S}_5\text{Br}$	8.73E-4	0.178	$\bar{\text{F}43m}$	216		234587	168
$\text{Li}_{6.1}\text{P}_{0.95}\text{Si}_{0.1}\text{S}_5\text{Br}$	7.99E-4	0.22	$\bar{\text{F}43m}$	216		234588	168
$\text{Li}_{6.125}\text{P}_{0.875}\text{Si}_{0.125}\text{S}_5\text{Br}$	9.02E-4	0.189	$\bar{\text{F}43m}$	216		234589	168
$\text{Li}_{6.175}\text{P}_{0.825}\text{Si}_{0.175}\text{S}_5\text{Br}$	9.31E-4	0.142	$\bar{\text{F}43m}$	216		234591	168
$\text{Li}_{6.2}\text{P}_{0.8}\text{Si}_{0.2}\text{S}_5\text{Br}$	1.69E-3	0.25	$\bar{\text{F}43m}$	216		234592	168
$\text{Li}_{6.225}\text{P}_{0.775}\text{Si}_{0.225}\text{S}_5\text{Br}$	1.08E-3	0.248	$\bar{\text{F}43m}$	216		234593	168
$\text{Li}_{6.25}\text{P}_{0.75}\text{Si}_{0.25}\text{S}_5\text{Br}$	1.41E-3	0.223	$\bar{\text{F}43m}$	216		234594	168
$\text{Li}_{6.3}\text{P}_{0.7}\text{Si}_{0.3}\text{S}_5\text{Br}$	1.65E-3	0.236	$\bar{\text{F}43m}$	216		234595	168
$\text{Li}_{6.35}\text{P}_{0.65}\text{Si}_{0.35}\text{S}_5\text{Br}$	2.34E-3	0.142	$\bar{\text{F}43m}$	216		234596	168
$\text{Li}_{6.5}\text{P}_{0.5}\text{Si}_{0.5}\text{S}_5\text{Br}$	2.19E-3	0.27	$\bar{\text{F}43m}$	216		234597	168
$\text{Li}_7\text{Ge}_3\text{PS}_{12}$	1.1E-4	0.259	$\bar{\text{F}43m}$	216		258187	169
$\text{Li}_6\text{B}_{0.9}\text{PH}_{3.6}\text{S}_{4.9}$	1.8E-3	0.166	$\bar{\text{F}43m}$	216		264526	170
$\text{Li}_6\text{PS}_5\text{Cl}$	1.30E-03	0.33	$\bar{\text{F}43m}$	216			171
$\text{Li}_6\text{PS}_5\text{Br}$	2.77E-3	0.31	$\bar{\text{F}43m}$	216		267193	172
$\text{Li}_6\text{P}(\text{S}_{4.9}\text{Se}_{0.1})\text{Br}$	3.20E-3	0.33	$\bar{\text{F}43m}$	216		267194	172
$\text{Li}_6\text{P}(\text{S}_{4.8}\text{Se}_{0.2})\text{Br}$	3.92E-3	0.34	$\bar{\text{F}43m}$	216		267195	172
$\text{Li}_6\text{P}(\text{S}_{4.7}\text{Se}_{0.3})\text{Br}$	3.62E-3	0.33	$\bar{\text{F}43m}$	216		267196	172
$\text{Li}_6\text{P}(\text{S}_{4.6}\text{Se}_{0.4})\text{Br}$	3.64E-3	0.33	$\bar{\text{F}43m}$	216		267197	172
$\text{Li}_6\text{P}(\text{S}_{4.5}\text{Se}_{0.5})\text{Br}$	2.68E-3	0.34	$\bar{\text{F}43m}$	216		267198	172
$\text{Li}_6\text{P}(\text{S}_{4.4}\text{Se}_{0.6})\text{Br}$	2.78E-3	0.34	$\bar{\text{F}43m}$	216		267199	172
$\text{Li}_6\text{P}(\text{S}_{4.3}\text{Se}_{0.7})\text{Br}$	3.01E-3	0.35	$\bar{\text{F}43m}$	216		267200	172
$\text{Li}_6\text{P}(\text{S}_{4.2}\text{Se}_{0.8})\text{Br}$	3.48E-3	0.34	$\bar{\text{F}43m}$	216		267201	172
$\text{Li}_6\text{P}(\text{S}_{4.1}\text{Se}_{0.9})\text{Br}$	3.82E-3	0.34	$\bar{\text{F}43m}$	216		267202	172

$\text{Li}_6\text{P}(\text{S}_4\text{Se})\text{Br}$	3.61E-3	0.34	F $\bar{4}$ 3m	216		267203	172
$\text{Li}_6\text{PO}_5\text{Cl}$	5.54E-10	0.66	F $\bar{4}$ 3m	216		421479	173
$\text{Li}_6\text{PS}_5\text{Br}$	3.2E-5	0.32	F $\bar{4}$ 3m	216		234598	174
$\text{Li}_6\text{PS}_5\text{Cl}$	3.3E-5	0.38	F $\bar{4}$ 3m	216		259205	174
$\text{Li}_6\text{PS}_5\text{I}$	2.2E-4	0.26	F $\bar{4}$ 3m	216		259212	174
$\text{Li}_6\text{PS}_5\text{I}$	1.26E-6	0.38	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.92}\text{Ge}_{0.08}\text{S}_5\text{I}$	9.02E-6	0.39	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.85}\text{Ge}_{0.15}\text{S}_5\text{I}$	3.99E-5	0.36	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.75}\text{Ge}_{0.25}\text{S}_5\text{I}$	3.26E-5	0.36	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.74}\text{Ge}_{0.26}\text{S}_5\text{I}$	1.51E-4	0.30	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.64}\text{Ge}_{0.36}\text{S}_5\text{I}$	6.58E-4	0.24	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.53}\text{Ge}_{0.47}\text{S}_5\text{I}$	1.52E-3	0.24	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.48}\text{Ge}_{0.52}\text{S}_5\text{I}$	1.83E-3	0.23	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.31}\text{Ge}_{0.69}\text{S}_5\text{I}$	5.16E-3	0.24	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{P}_{0.21}\text{Ge}_{0.79}\text{S}_5\text{I}$	5.41E-3	0.25	F $\bar{4}$ 3m	216			175
$\text{Li}_6\text{PS}_5\text{Cl}$	1.31E-6	0.38	F $\bar{4}$ 3m	216			176
$\text{Li}_6\text{PS}_5\text{Br}$	2.41E-5	0.16	F $\bar{4}$ 3m	216		259208	176
$\text{Li}_6\text{PS}_5\text{I}$	4.1E-7	0.32	F $\bar{4}$ 3m	216		418489	176
$\text{Li}_6\text{PS}_5\text{I}$	9.24E-5		F $\bar{4}$ 3m	216			177
$\text{Li}_{6.1}\text{P}_{0.9}\text{Sn}_{0.1}\text{S}_5\text{I}$	1.61E-4		F $\bar{4}$ 3m	216			177
$\text{Li}_{6.2}\text{P}_{0.8}\text{Sn}_{0.2}\text{S}_5\text{I}$	2.32E-4		F $\bar{4}$ 3m	216			177
$\text{Li}_{6.25}\text{P}_{0.75}\text{Sn}_{0.25}\text{S}_5\text{I}$	2.92E-4		F $\bar{4}$ 3m	216			177
$\text{Li}_{6.3}\text{P}_{0.7}\text{Sn}_{0.3}\text{S}_5\text{I}$	3.06E-4		F $\bar{4}$ 3m	216			177
$\text{Li}_{6.5}\text{P}_{0.5}\text{Sn}_{0.5}\text{S}_5\text{I}$	2.35E-4		F $\bar{4}$ 3m	216			177
$\text{Li}_{6.4}\text{P}_{0.6}\text{Ge}_{0.4}\text{S}_5\text{I}$	2.51E-4		F $\bar{4}$ 3m	216			177

$\text{Li}_{6.45}\text{P}_{0.55}\text{Ge}_{0.45}\text{S}_5\text{I}$	3.65E-4		F $\bar{4}3m$	216			177
$\text{Li}_{6.5}\text{P}_{0.5}\text{Ge}_{0.5}\text{S}_5\text{I}$	5.42E-4		F $\bar{4}3m$	216			177
$\text{Li}_{6.55}\text{P}_{0.45}\text{Ge}_{0.55}\text{S}_5\text{I}$	4.11E-4		F $\bar{4}3m$	216			177
$\text{Li}_{6.6}\text{P}_{0.4}\text{Ge}_{0.6}\text{S}_5\text{I}$	2.74E-4		F $\bar{4}3m$	216			177
$\text{Li}_{6.8}\text{P}_{0.2}\text{Ge}_{0.8}\text{S}_5\text{I}$	5.21E-5		F $\bar{4}3m$	216			177
$\text{LiCe}(\text{BH}_4)_3\text{Cl}$	1.03E-4		I $\bar{4}3m$	217		185218	178
Li_7PN_4	1.60E-07	0.4	P $\bar{4}3n$	218		69017	95
$\beta\text{-Li}_8\text{GeP}_4$	8.6E-5	0.394	P $\bar{4}3n$	218	$\beta\text{-Li}_8\text{GeP}_4$	235185	161
$\text{Li}_4\text{B}_7\text{O}_{12}\text{Cl}$	2.4E-5		F $\bar{4}3c$	219		1125	179
$\text{Fe}_{0.16}\text{La}_{2.95}\text{Li}_{5.68}\text{Zr}_2\text{O}_{12}$	9.35E-4	0.29	I $\bar{4}3d$	220		431391	180
$\text{Fe}_{0.19}\text{La}_{2.95}\text{Li}_{5.57}\text{Zr}_2\text{O}_{12}$	1.38E-3	0.28	I $\bar{4}3d$	220		431392	180
Li_3ClO	2.5E-2		Pm $\bar{3}m$	221			181
$\text{Li}_{2.99}\text{Ba}_{0.005}\text{Cl}_{0.5}\text{I}_{0.5}$	2.5E-3	0.06	Pm $\bar{3}m$	221			181
$\text{Li}_{0.31}\text{La}_{0.63}((\text{Ti}_{0.9}\text{Co}_{0.1})\text{O}_3)$	2.60E-4		Pm $\bar{3}m$	221		151533	182
$(\text{La}_{0.49}\text{Li}_{0.461}\text{Sr}_{0.049})(\text{TiO}_3)$	7.09E-4	0.33	Pm $\bar{3}m$	221		190825	183
$(\text{La}_{0.46}\text{Li}_{0.429}\text{Sr}_{0.111})(\text{TiO}_3)$	1.97E-4	0.33	Pm $\bar{3}m$	221		190826	183
$(\text{La}_{0.402}\text{Li}_{0.368}\text{Sr}_{0.230})(\text{TiO}_3)$	2.87E-5	0.36	Pm $\bar{3}m$	221		190827	183
$\text{Li}_2(\text{OH})_{0.9}\text{F}_{0.1}\text{Cl}$	3.86E-5	0.52	Pm $\bar{3}m$	221			184
$\text{Li}_2(\text{OH})\text{Br}$	1.20E-6	0.75	Pm $\bar{3}m$	221		200874	184
Li_9NS_3	8.30E-07	0.52	Pm $\bar{3}m$	221		240749	185
$(\text{La}_{0.55}\text{Li}_{0.45})(\text{Ti}_{0.9}\text{Al}_{0.1})\text{O}_3$	1.51E-3		Pm $\bar{3}m$	221		254045	186
$(\text{La}_{0.6}\text{Li}_{0.4})(\text{Ti}_{0.8}\text{Al}_{0.2})\text{O}_3$	5.68E-4		Pm $\bar{3}m$	221		254046	186
$(\text{La}_{0.65}\text{Li}_{0.35})(\text{Ti}_{0.7}\text{Al}_{0.3})\text{O}_3$	1.61E-4		Pm $\bar{3}m$	221		254047	186

(La _{0.7} Li _{0.3})(Ti _{0.6} Al _{0.4})O ₃	1.04E-7		Pm $\bar{3}$ m	221		254048	186
(Li _{0.16} Sr _{0.69})(Ga _{0.25} Ta _{0.75})O ₃	3.69E-6	0.359	Pm $\bar{3}$ m	221		291520	187
Li _{0.375} Sr _{0.4375} Zr _{0.25} Ta _{0.75} O ₃	2.0E-4	0.26	Pm $\bar{3}$ m	221			188
Li _{0.25} Sr _{0.625} Ta _{0.5} Zr _{0.5} O ₃	3.34E-7	0.42	Pm $\bar{3}$ m	221			188
Li _{0.375} Sr _{0.4375} Hf _{0.25} Ta _{0.75} O ₃	3.8E-4	0.36	Pm $\bar{3}$ m	221			189
Li _{0.375} Sr _{0.4375} Zr _{0.25} Nb _{0.75} O ₃	2.00E-5	0.26	Pm $\bar{3}$ m	221			190
Li _{0.25} Sr _{0.625} Zr _{0.5} Nb _{0.5} O ₃	2.75E-7	0.36	Pm $\bar{3}$ m	221			190
Li _{2.99} Ba _{0.005} ClO	2.5E-2	0.13	Pm $\bar{3}$ m	221			191
Li _{2.99} Ba _{0.005} Cl _{0.5} I _{0.5} O	3.37E-3		Pm $\bar{3}$ m	221			191
Sm _{0.5} Li _{0.42} TiO _{2.96}	3.93E-10	0.58	Pm $\bar{3}$ m	221			86
La _{0.52} Li _{0.35} TiO _{2.96}	9.11E-4	0.32	Pm $\bar{3}$ m	221			86
La _{0.61} Li _{0.15} TiO ₃	2.06E-4		Pm $\bar{3}$ m	221			192
La _{0.58} Li _{0.24} TiO ₃	7.22E-4		Pm $\bar{3}$ m	221			192
La _{0.55} Li _{0.33} TiO ₃	1.58E-3		Pm $\bar{3}$ m	221			192
La _{0.54} Li _{0.36} TiO ₃	9.79E-3		Pm $\bar{3}$ m	221			192
La _{0.52} Li _{0.42} TiO ₃	7.21E-4		Pm $\bar{3}$ m	221			192
La _{0.6} Sr _{0.06} Li _{0.06} TiO ₃	1.13E-5	0.37	Pm $\bar{3}$ m	221			193
La _{0.56} Sr _{0.1} Li _{0.1} TiO ₃	1.37E-5	0.37	Pm $\bar{3}$ m	221			193
La _{0.51} Sr _{0.15} Li _{0.15} TiO ₃	5.3E-5	0.38	Pm $\bar{3}$ m	221			193
La _{0.41} Sr _{0.25} Li _{0.25} TiO ₃	7.64E-5	0.35	Pm $\bar{3}$ m	221			193
La _{0.385} Sr _{0.275} Li _{0.275} TiO ₃	6.04E-5	0.37	Pm $\bar{3}$ m	221			193
La _{0.36} Sr _{0.3} Li _{0.3} TiO ₃	1.92E-5	0.35	Pm $\bar{3}$ m	221			193
La _{0.61} Li _{0.18} TiO ₃	2.09E-4		Pm $\bar{3}$ m	221			97

La _{0.58} Li _{0.27} TiO ₃	8.32E-4		Pm $\bar{3}$ m	221			97
La _{0.56} Li _{0.33} TiO ₃	1.30E-3		Pm $\bar{3}$ m	221			97
La _{0.55} Li _{0.36} TiO ₃	1.54E-3	0.33	Pm $\bar{3}$ m	221			97
La _{0.54} Li _{0.39} TiO ₃	1.25E-3		Pm $\bar{3}$ m	221			97
La _{0.52} Li _{0.45} TiO ₃	7.85E-4		Pm $\bar{3}$ m	221			97
La _{0.51} Li _{0.34} TiO _{2.94}	7E-5	0.36	Pm $\bar{3}$ m	221			62
Li ₃ OBr	1.10E-06	0.74	Pm $\bar{3}$ m	221		67265	194,195
Li _{7.2} N _{1.6} Cl _{2.4}	8.4E-7	0.49	Fm $\bar{3}$ m	225		49646	131
Li ₆ Ni ₃	3.70E-06		Fm $\bar{3}$ m	225		83380	165
Li _{0.19} La _{0.67} (Ti _{0.9} Co _{0.1})O ₃	1.08E-4		Fm $\bar{3}$ m	225		151535	182
Li ₆ NBr ₃	1.00E-08	0.69	Fm $\bar{3}$ m	225		84091	196
Lil	1E-7		Fm $\bar{3}$ m	225		414244	197
Li(Li _{0.34} Ti _{1.66})O ₄	6.03E-8	0.506	Fd $\bar{3}$ m	227		168137	164
(Li _{0.916} Mg _{0.084})(Li _{0.352} Mg _{0.016} Ti _{1.634})O ₄	1.73E-8	0.564	Fd $\bar{3}$ m	227		168139	164
(Li _{0.826} Mg _{0.174})(Li _{0.374} Mg _{0.026} Ti _{1.60})O ₄	4.24E-9	0.615	Fd $\bar{3}$ m	227		168141	164
(Li _{0.74} Mg _{0.26})(Li _{0.40} Mg _{0.04} Ti _{1.56})O ₄	1.51E-9	0.639	Fd $\bar{3}$ m	227		168142	164
Li ₂ MnCl ₄	4.79E-6		Fd $\bar{3}$ m	227		69678	166
Li ₂ MgCl ₄	6.24E-7		Fd $\bar{3}$ m	227		74957	166
Li _{1.9} Mn _{0.9} Ga _{0.1} Cl ₄	2.37E-7		Fd $\bar{3}$ m	227		50305	198
Li _{1.65} Mn _{0.65} In _{0.35} Cl ₄	9.9E-8		Fd $\bar{3}$ m	227		50306	198
LiCdCl ₄	5.80E-07	0.44	Fd $\bar{3}$ m	227		74958	199
LiSrNb ₂ O ₆ F	<1E-10	0.604	Fd $\bar{3}$ m	227		236009	200
LiSrTa ₂ O ₆ F	<1E-10	0.604	Fd $\bar{3}$ m	227		236010	200

$\text{LiSr}_{0.9}\text{Nb}_2\text{O}_6\text{F}_{0.8}$	<1E-10	0.709	Fd $\bar{3}$ m	227		236011	200
$\text{LiSr}_{0.9}\text{Ta}_2\text{O}_6\text{F}_{0.8}$	<1E-10	0.76	Fd $\bar{3}$ m	227		236012	200
$\text{Li}_{1.1}\text{SrNb}_{1.9}\text{Zr}_{0.1}\text{O}_6\text{F}$	<1E-10	0.622	Fd $\bar{3}$ m	227		236013	200
$\text{Li}_{1.1}\text{SrTa}_{1.9}\text{Zr}_{0.1}\text{O}_6\text{F}$	<1E-10	0.693	Fd $\bar{3}$ m	227		236014	200
$\text{Li}_6\text{SrLa}_2\text{Nb}_2\text{O}_{12}$	4.2E-6	0.5	la $\bar{3}$ d	230		157628	159
$\text{Li}_6\text{CaLa}_2\text{Nb}_2\text{O}_{12}$	1.6E-6	0.55	la $\bar{3}$ d	230		161386	159
$\text{Li}_{5.25}\text{Ba}_{0.25}\text{La}_{2.75}\text{Ta}_2\text{O}_{12}$	6.03E-6	0.479	la $\bar{3}$ d	230			201
$\text{Li}_{5.5}\text{Ba}_{0.5}\text{La}_{2.5}\text{Ta}_2\text{O}_{12}$	1.35E-5	0.455	la $\bar{3}$ d	230			201
$\text{Li}_{6.25}\text{Ba}_{1.25}\text{La}_{1.75}\text{Ta}_2\text{O}_{12}$	5.05E-5	0.395	la $\bar{3}$ d	230			201
$\text{Li}_{6.5}\text{Ba}_{1.5}\text{La}_{1.5}\text{Ta}_2\text{O}_{12}$	3.2E-5	0.402	la $\bar{3}$ d	230			201
$\text{Li}_{6.75}\text{Ba}_{1.75}\text{La}_{1.25}\text{Ta}_2\text{O}_{12}$	1.25E-5	0.418	la $\bar{3}$ d	230			201
$\text{Li}_7\text{Ba}_2\text{LaTa}_2\text{O}_{12}$	3.00E-6	0.442	la $\bar{3}$ d	230			201
$\text{Li}_5\text{La}_3\text{Ta}_2\text{O}_{12}$	4.33E-6	0.50	la $\bar{3}$ d	230		154400	201
$\text{Li}_6\text{BaLa}_2\text{Ta}_2\text{O}_{12}$	3.02E-5	0.419	la $\bar{3}$ d	230		237201	201
$\text{Li}_7\text{La}_3\text{Zr}_{1.89}\text{Al}_{0.15}\text{O}_{12}$	3.4E-4	0.334	la $\bar{3}$ d	230			202
$\text{Li}_{7.06}\text{La}_3\text{Y}_{0.06}\text{Zr}_{1.94}\text{O}_{12}$	9.56E-4	0.26	la $\bar{3}$ d	230			203
$\text{Li}_{6.25}\text{La}_3\text{Zr}_2\text{Ga}_{0.25}\text{O}_{12}$	3.5E-4		la $\bar{3}$ d	230			204
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.2E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.8}\text{La}_3\text{Zr}_{1.8}\text{Ta}_{0.2}\text{O}_{12}$	2.8E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.6}\text{La}_3\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	7.3E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.5}\text{Ta}_{0.5}\text{O}_{12}$	9.2E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.6}\text{O}_{12}$	1.0E-3	0.35	la $\bar{3}$ d	230			205
$\text{Li}_{6.2}\text{La}_3\text{Zr}_{1.2}\text{Ta}_{0.8}\text{O}_{12}$	3.2E-4		la $\bar{3}$ d	230			205
$\text{Li}_6\text{La}_3\text{ZrTaO}_{12}$	1.6E-4		la $\bar{3}$ d	230			205
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.2E-4		la $\bar{3}$ d	230			205

$\text{Li}_{6.8}\text{La}_3\text{Zr}_{1.8}\text{Ta}_{0.2}\text{O}_{12}$	2.8E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.6}\text{La}_3\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	7.3E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.5}\text{Ta}_{0.5}\text{O}_{12}$	9.2E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.6}\text{O}_{12}$	1E-3	0.35	la $\bar{3}$ d	230			205
$\text{Li}_{6.2}\text{La}_3\text{Zr}_{1.2}\text{Ta}_{0.8}\text{O}_{12}$	3.2E-4		la $\bar{3}$ d	230			205
$\text{Li}_6\text{La}_3\text{ZrTaO}_{12}$	1.6E-4		la $\bar{3}$ d	230			205
$\text{Li}_{6.8}\text{La}_3\text{Zr}_{1.8}\text{Ta}_{0.2}\text{O}_{12}$	7.8E-4		la $\bar{3}$ d	230			206
$\text{Li}_{6.75}\text{La}_3\text{Zr}_{1.75}\text{Ta}_{0.25}\text{O}_{12}$	8.8E-4		la $\bar{3}$ d	230			206
$\text{Li}_{6.65}\text{La}_3\text{Zr}_{1.65}\text{Ta}_{0.35}\text{O}_{12}$	7.7E-4		la $\bar{3}$ d	230			206
$\text{Li}_{6.6}\text{La}_3\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	7.2E-4		la $\bar{3}$ d	230			206
$\text{Li}_{6.55}\text{La}_3\text{Zr}_{1.55}\text{Ta}_{0.45}\text{O}_{12}$	6.9E-4		la $\bar{3}$ d	230			206
$\text{Li}_6\text{La}_3\text{ZrTaO}_{12}$	4.4E-4		la $\bar{3}$ d	230			206
$\text{Li}_5\text{La}_3\text{Ta}_2\text{O}_{12}$	1.6E-4		la $\bar{3}$ d	230			206
$\text{Li}_{6.7}\text{La}_3\text{Zr}_{1.7}\text{Ta}_{0.3}\text{O}_{12}$	9.6E-4	0.37	la $\bar{3}$ d	230			206
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.5}\text{Ta}_{0.5}\text{O}_{12}$	6.7E-4		la $\bar{3}$ d	230		183686	206
$\text{Li}_{6.05}\text{Ga}_{0.25}\text{La}_3\text{Zr}_2\text{O}_{11.8}\text{F}_{0.2}$	1.28E-3	0.28	la $\bar{3}$ d	230			207
$\text{Li}_{5.72}\text{Al}_{0.26}\text{La}_3\text{Zr}_{1.5}\text{W}_{0.25}\text{O}_{12}$	4.9E-4	0.35	la $\bar{3}$ d	230			208
$\text{Li}_{6.8}\text{La}_3\text{Zr}_{1.9}\text{Mo}_{0.1}\text{O}_{12}$	8.00E-5	0.46	la $\bar{3}$ d	230			209
$\text{Li}_{6.6}\text{La}_3\text{Zr}_{1.8}\text{Mo}_{0.2}\text{O}_{12}$	3.11E-4	0.48	la $\bar{3}$ d	230			209
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.7}\text{Mo}_{0.3}\text{O}_{12}$	3.69E-4	0.49	la $\bar{3}$ d	230			209
$\text{Li}_{6.2}\text{La}_3\text{Zr}_{1.6}\text{Mo}_{0.4}\text{O}_{12}$	3.40E-4	0.48	la $\bar{3}$ d	230			209
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.75}\text{Mo}_{0.25}\text{O}_{12}$	3.33E-4	0.39	la $\bar{3}$ d	230		239128	209
$\text{Li}_{6.75}\text{La}_3\text{Zr}_{1.875}\text{Te}_{0.125}\text{O}_{12}$	3.30E-4	0.41	la $\bar{3}$ d	230			210
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.75}\text{Te}_{0.25}\text{O}_{12}$	1.02E-3	0.38	la $\bar{3}$ d	230			210

$\text{Li}_{6.375}\text{La}_3\text{Zr}_{1.375}\text{Nb}_{0.625}\text{O}_2$	1.37E-3	0.25	la $\bar{3}$ d	230			211
$\text{Li}_5\text{La}_3\text{Ta}_2\text{O}_{12}$	1.2E-6	0.56	la $\bar{3}$ d	230		154400	212
$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	1E-5	0.43	la $\bar{3}$ d	230		171171	212
$\text{Li}_5\text{La}_3\text{Bi}_2\text{O}_{12}$	4.00E-05	0.47	la $\bar{3}$ d	230		158372	213
$\text{Li}_6\text{La}_2\text{SrBi}_2\text{O}_{12}$	5.20E-05	0.43	la $\bar{3}$ d	230		158373	213
$\text{Li}_5\text{Nd}_3\text{Sb}_2\text{O}_{12}$	1.3E-7	0.67	la $\bar{3}$ d	230		159426	214
$\text{Li}_4\text{Nd}_3\text{TeSbO}_{12}$	1.96E-6	0.64	la $\bar{3}$ d	230		159732	215
$\text{Li}_5\text{La}_3\text{Sb}_2\text{O}_{12}$	8.2E-6	0.51	la $\bar{3}$ d	230		161342	216
$\text{Li}_6\text{SrLa}_2\text{Sb}_2\text{O}_{12}$	6.6E-6	0.54	la $\bar{3}$ d	230		161343	216
$\text{Li}_6(\text{La}_2\text{Ca})(\text{NbO}_6)_2$	1.33E-6		la $\bar{3}$ d	230		161386	217
$\text{Li}_6(\text{La}_2\text{Sr})(\text{NbO}_6)_2$	3.69E-6		la $\bar{3}$ d	230		161387	217
$\text{Li}_6\text{CaLa}_2\text{Ta}_2\text{O}_{12}$	2.2E-6	0.5	la $\bar{3}$ d	230		163860	218
$\text{Li}_6\text{BaLa}_2\text{Ta}_2\text{O}_{12}$	1.3E-5	0.44	la $\bar{3}$ d	230		163861	218
$\text{Li}_{6.15}\text{La}_3\text{Zr}_{1.75}\text{Ta}_{0.25}\text{Ga}_{0.2}\text{O}_{12}$	4.1E-4	0.27	la $\bar{3}$ d	230			219
$\text{Li}_{6.15}\text{La}_3\text{Zr}_{1.75}\text{Ta}_{0.25}\text{Al}_{0.2}\text{O}_{12}$	3.7E-4	0.30	la $\bar{3}$ d	230			219
$\text{Li}_{6.75}\text{La}_3\text{Zr}_{1.75}\text{Ta}_{0.25}\text{O}_{12}$	8.7E-4	0.22	la $\bar{3}$ d	230		183873	219
$\text{Li}_{6.16}\text{Al}_{0.28}\text{La}_3\text{Zr}_2\text{O}_{12}$	6.1E-4	0.34	la $\bar{3}$ d	230		185539	220
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.97E-6	0.49	la $\bar{3}$ d	230			221
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}\text{-}0.5\text{wt\% Al}$	1.58E-4		la $\bar{3}$ d	230			221
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}\text{-}0.9\text{wt\% Al}$	3.2E-4	0.34	la $\bar{3}$ d	230			221
$\text{Li}_{6.06}\text{Al}_{0.2}\text{La}_3\text{Zr}_2\text{O}_{12}$	4E-4	0.34	la $\bar{3}$ d	230		185539	221
$\text{Li}_6\text{BaLa}_2\text{Ta}_2\text{O}_{12}$	2.45E-5	0.40	la $\bar{3}$ d	230		185602	222
$\text{Nd}_3\text{Zr}_2\text{Al}_{0.5}\text{Li}_{5.5}\text{O}_{12}$	3.9E-5	0.56	la $\bar{3}$ d	230		189530	223

(Li _{6.26} Al _{0.24})La ₃ Zr ₂ O ₁₂	3.1E-4	0.33	la $\bar{3}$ d	230		195182	224
Li ₆ La ₃ Nb _{1.5} Y _{0.5} O ₁₂	1.88E-4		la $\bar{3}$ d	230		237141	225
Li _{5.2} La ₃ Nb _{1.9} Y _{0.1} O ₁₂	6.39E-5		la $\bar{3}$ d	230		237143	225
Li _{5.4} La ₃ Nb _{1.8} Y _{0.2} O ₁₂	6.74E-5		la $\bar{3}$ d	230		237144	225
Li _{5.5} La ₃ Nb _{1.75} Y _{0.25} O ₁₂	9.18E-5		la $\bar{3}$ d	230		237145	225
Li _{6.5} La ₃ Nb _{1.25} Y _{0.75} O ₁₂	3.43E-4		la $\bar{3}$ d	230		237146	225
Li ₆ Ba _{0.5} Sr _{0.5} La ₂ Ta ₂ O ₁₂	7.1E-6	0.45	la $\bar{3}$ d	230		237199	226
Li ₆ SrLa ₂ Ta ₂ O ₁₂	5.4E-6	0.45	la $\bar{3}$ d	230		237200	226
Li ₆ BaLa ₂ Ta ₂ O ₁₂	1.5E-5	0.47	la $\bar{3}$ d	230		237201	226
Li ₆ CaLa ₂ Ta ₂ O ₁₂	2.2E-6	0.47	la $\bar{3}$ d	230		237202	226
Li ₆ BaLa ₂ Ta ₂ O ₁₂	4E-5	0.4	la $\bar{3}$ d	230			227
Li ₆ SrLa ₂ Ta ₂ O ₁₂	7E-6	0.5	la $\bar{3}$ d	230			227
Li ₆ SrLa ₂ Ta ₂ O ₁₂	7E-6	0.5	la $\bar{3}$ d	230		237200	227
Li ₆ BaLa ₂ Ta ₂ O ₁₂	4E-5	0.4	la $\bar{3}$ d	230		237201	227
Li _{5.74} La ₃ Zr _{1.5} Ta _{0.5} O ₁₂	9.03E-4	0.435	la $\bar{3}$ d	230		239663	228
La ₃ Li _{5.08} Ta _{1.51} Zr _{0.39} O ₁₂	1.03E-4	0.536	la $\bar{3}$ d	230		239664	228
Li _{51.2} Al _{1.6} La ₂₄ Zr ₁₆ O ₉₆	2.54E-4	0.36	la $\bar{3}$ d	230		241475	229
Li _{49.6} Al _{1.6} La ₂₄ Zr _{14.4} Ta _{1.6} O ₉₆	6.14E-4	0.29	la $\bar{3}$ d	230		241476	229
Li _{6.5} La ₃ Hf _{1.5} Ta _{0.5} O ₁₂	4.0E-4	0.40	la $\bar{3}$ d	230		258921	230
Li _{6.5} La ₃ Sn _{1.5} Ta _{0.5} O ₁₂	1.9E-4	0.45	la $\bar{3}$ d	230		258922	230
Li ₅ La ₃ Ta ₂ O ₁₂	1.59E-5		la $\bar{3}$ d	230		259164	231
Li _{5.3} La ₃ Ta _{1.85} Sm _{0.15} O ₁₂	7.11E-6		la $\bar{3}$ d	230		259165	231
Li _{5.5} La ₃ Ta _{1.75} Sm _{0.25} O ₁₂	5.17E-6		la $\bar{3}$ d	230		259166	231
Li _{5.70} La ₃ Ta _{1.65} Sm _{0.35} O ₁₂	2.15E-5		la $\bar{3}$ d	230		259167	231

$\text{Li}_{5.90}\text{La}_3\text{Ta}_{1.55}\text{Sm}_{0.45}\text{O}_{12}$	1.18E-5		la $\bar{3}$ d	230		259168	231
$\text{Li}_{6.10}\text{La}_3\text{Ta}_{1.45}\text{Sm}_{0.55}\text{O}_{12}$	1.40E-5		la $\bar{3}$ d	230		259169	231
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	5.69E-04	0.36	la $\bar{3}$ d	230	"cubic LLZO"	422259	232
$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	4.99e-6		la $\bar{3}$ d	230			233
$\text{Li}_5\text{La}_3\text{Nb}_{1.95}\text{Y}_{0.05}\text{O}_{12}$	1.32E-5		la $\bar{3}$ d	230			233
$\text{Li}_5\text{La}_3\text{Nb}_{1.9}\text{Y}_{0.1}\text{O}_{12}$	1.43E-5		la $\bar{3}$ d	230			233
$\text{Li}_5\text{La}_3\text{Nb}_{1.85}\text{Y}_{0.15}\text{O}_{12}$	5.85E-6		la $\bar{3}$ d	230			233
$\text{Li}_5\text{La}_3\text{Nb}_{1.8}\text{Y}_{0.2}\text{O}_{12}$	9.05E-6		la $\bar{3}$ d	230			233
$\text{Li}_5\text{La}_3\text{Nb}_{1.75}\text{Y}_{0.25}\text{O}_{12}$	9.42E-6		la $\bar{3}$ d	230			233
$\text{Li}_{6.24}\text{La}_3\text{Zr}_2\text{Al}_{0.24}\text{O}_{11.98}$	4.0E-4	0.26	la $\bar{3}$ d	230			234
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}\text{-}0.3\text{Ga}$	3.8E-5	0.37	la $\bar{3}$ d	230			235
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}\text{-}0.4\text{Ga}$	4.4E-5	0.36	la $\bar{3}$ d	230			235
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}\text{-}0.5\text{Ga}$	8.9E-5	0.36	la $\bar{3}$ d	230			235
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}\text{-Ga}$	5.4E-4	0.32	la $\bar{3}$ d	230			235
$\text{La}_3\text{Zr}_2\text{Ga}_{0.5}\text{Li}_{5.5}\text{O}_{12}$	1E-4		la $\bar{3}$ d	230			236
$\text{Li}_{6.8}\text{La}_3\text{Zr}_{1.8}\text{Sb}_{0.2}\text{O}_{12}$	5.9E-5	0.39	la $\bar{3}$ d	230			237
$\text{Li}_{6.6}\text{La}_3\text{Zr}_{1.6}\text{Sb}_{0.4}\text{O}_{12}$	7.7E-4	0.34	la $\bar{3}$ d	230			237
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Sb}_{0.6}\text{O}_{12}$	6.6E-4	0.36	la $\bar{3}$ d	230			237
$\text{Li}_{6.2}\text{La}_3\text{Zr}_{1.2}\text{Sb}_{0.8}\text{O}_{12}$	4.5E-4	0.37	la $\bar{3}$ d	230			237
$\text{Li}_6\text{La}_3\text{ZrSbO}_{12}$	2.6E-4	0.38	la $\bar{3}$ d	230			237
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.75}\text{Te}_{0.25}\text{O}_{12}\text{-}0.07\text{Al}$	4E-4	0.33	la $\bar{3}$ d	230			238
$\text{Li}_{6.65}\text{La}_{2.75}\text{Ba}_{0.25}\text{Zr}_{1.4}\text{Ta}_{0.5}\text{Nb}_{0.1}\text{O}_{12}$	5.27E-4	0.26	la $\bar{3}$ d	230			239
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.6}\text{O}_{12}$	7.24E-4	0.24	la $\bar{3}$ d	230			239

$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.5}\text{Nb}_{0.1}\text{O}_2$	4.44E-4	0.27	la $\bar{3}$ d	230			239
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.4}\text{Nb}_{0.2}\text{O}_2$	4.55E-4	0.28	la $\bar{3}$ d	230			239
$\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.3}\text{Nb}_{0.3}\text{O}_2$	6.06E-4	0.26	la $\bar{3}$ d	230			239
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.74E-4	0.26	la $\bar{3}$ d	230			239
$\text{Li}_3\text{Nd}_3\text{Te}_2\text{O}_{12}$	<1E-10	1.22	la $\bar{3}$ d	230			240
$\text{Li}_{7.131}\text{La}_3\text{Zr}_2\text{O}_{12}\text{Al}_{0.244}$	7.73E-5		la $\bar{3}$ d	230			241
$\text{Li}_{6.949}\text{La}_3\text{Zr}_2\text{O}_{12}\text{Al}_{0.262}$	2.25E-4		la $\bar{3}$ d	230			241
$\text{Li}_{6.835}\text{La}_3\text{Zr}_2\text{O}_{12}\text{Al}_{0.231}$	2.20E-4		la $\bar{3}$ d	230			241
$\text{Li}_{6.660}\text{La}_3\text{Zr}_2\text{O}_{12}\text{Al}_{0.258}$	1.51E-4		la $\bar{3}$ d	230			241
$\text{Li}_{6.75}\text{La}_3\text{Zr}_{1.75}\text{Ta}_{0.25}\text{O}_{12}$	4.1E-4	0.42	la $\bar{3}$ d	230			121
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.5}\text{Ta}_{0.5}\text{O}_{12}$	6.1E-4	0.4	la $\bar{3}$ d	230			121
$\text{Li}_6\text{La}_3\text{ZrTaO}_{12}$	2.1E-4	0.42	la $\bar{3}$ d	230			121
$\text{Li}_3\text{Gd}_3\text{Te}_2\text{O}_{12}$	<1E-10		la $\bar{3}$ d	230			242
$\text{Li}_3\text{Tb}_3\text{Te}_2\text{O}_{12}$	<1E-10		la $\bar{3}$ d	230			242
$\text{Li}_3\text{Er}_3\text{Te}_2\text{O}_{12}$	<1E-10		la $\bar{3}$ d	230			242
$\text{Li}_3\text{Lu}_3\text{Te}_2\text{O}_{12}$	<1E10		la $\bar{3}$ d	230			242
$\text{Li}_2\text{S}^*\text{P}_2\text{S}_5$	3.2E-03						4
0.7 Li_2S -0.3 P_2S_5	5.4E-5						4
$\text{Li}_{3.8}\text{Ge}_{0.8}\text{P}_{0.2}\text{S}_4$	1.75E-6	0.466					14
$\text{Li}_{3.6}\text{Ge}_{0.6}\text{P}_{0.4}\text{S}_4$	1.74E-4	0.339					14
$\text{Li}_{3.4}\text{Ge}_{0.4}\text{P}_{0.6}\text{S}_4$	6.53E-4	0.275					14
$\text{Li}_{3.35}\text{Ge}_{0.35}\text{P}_{0.65}\text{S}_4$	1.53E-3	0.229					14
$\text{Li}_{3.3}\text{Ge}_{0.3}\text{P}_{0.7}\text{S}_4$	1.76E-3	0.221					14

$\text{Li}_{3.2}\text{Ge}_{0.2}\text{P}_{0.8}\text{S}_4$	5.57E-4	0.275					14
$\text{Li}_{2.9}\text{Ca}_{0.05}\text{InBr}_6$	2.16E-4						25
$\text{Li}_{2.86}\text{Ca}_{0.07}\text{InBr}_6$	4.04E-4						25
$\text{Li}_{2.8}\text{Ca}_{0.1}\text{InBr}_6$	3.00E-4						25
$\text{Li}_{2.7}\text{Ca}_{0.15}\text{InBr}_6$	6.97E-5						25
$\text{Li}_{3.9}\text{Zn}_{0.05}\text{GeS}_4$	2.72E-7	0.517					71
$\text{Li}_{3.8}\text{Zn}_{0.1}\text{GeS}_4$	9.95E-8	0.545					71
$\text{Li}_{3.6}\text{Zn}_{0.2}\text{GeS}_4$	5.90E-8	0.539					71
Li_2GeS_3	9.7E-9						71
$\text{Li}_2\text{ZnGeS}_4$	1.4E-9						71
$\text{Li}_{9.6}\text{P}_3\text{S}_{12}$	1.2E-3	0.259					102
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ge}_{1.7}(\text{PO}_4)_3$	8.24E-5	0.386					133
$\text{Li}_{1.6}\text{Al}_{0.6}\text{Ge}_{1.4}(\text{PO}_4)_3$	2.84E-4	0.430					133
$\text{LiTi}_2(\text{PO}_4)_3\text{-}0.2\text{Li}_2\text{O}$	2.4E-4						134
$\text{LiTi}_2(\text{PO}_4)_3\text{-}0.3\text{Li}_2\text{O}$	1.5E-3						134
$\text{LiTi}_2(\text{PO}_4)_3\text{-}0.4\text{Li}_2\text{O}$	1.3E-4						134
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3\text{-}0.3\text{Li}_2\text{O}$	3.5E-4						134
$\text{LiTi}_2(\text{PO}_4)_3\text{-}0.1\text{Li}_4\text{P}_2\text{O}_7$	1.6E-4						134
$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	3.38E-3	0.30			LATP		243
$\text{Li}_{1.2}\text{Ge}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	7.94E-5	0.27			LAGP		243
$\text{Li}_{1.5}\text{Ge}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	1.90E-4	0.33			LAGP		243
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	3.38E-3	0.28			LATP	427619	243
Li_3ClO	0.85E-3	0.26					194
$\text{Li}_3\text{Cl}_{0.5}\text{Br}_{0.5}\text{O}$	1.94E-3	0.18					194
Li_3OCl	1.47E-4	0.26					194

$\text{Li}_3\text{OCl}_{0.5}\text{Br}_{0.5}$	9.49E-4	0.18						194
$\text{Li}_{6.6}\text{La}_{2.6}\text{Ce}_{0.4}\text{Zr}_2\text{O}_{12}$	1.44E-5	0.48						244
$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	1.1E-03							245
$80\text{Li}_2\text{S} * 20\text{P}_2\text{S}_5$	7.2E-04							246
$0.8\text{Li}_2\text{S}-0.2\text{P}_2\text{S}_5$	7.2E-4							246
$0.75\text{Li}_2\text{S}-0.25\text{P}_2\text{S}_5$	2.8E-4							246
$\text{Li}_2\text{S}^*\text{P}_2\text{S}_5^*\text{P}_2\text{S}_3$	5.4E-03							247
$\text{Li}_2\text{S}^*\text{P}_2\text{S}_5^*\text{Li}_3\text{N}$	1.4E-03							248
$\text{Li}_5\text{La}_3\text{Nb}_{1.9}\text{Y}_{0.1}\text{O}_{12}$	1.44E-5	0.55						233
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	2.35E-4	0.339						249
$\text{Li}_{6.88}\text{La}_3\text{Zr}_{1.88}\text{Nb}_{0.12}\text{O}_{12}$	5.99E-4	0.319						249
$\text{Li}_{6.75}\text{La}_3\text{Zr}_{1.75}\text{Nb}_{0.25}\text{O}_{12}$	7.71E-4	0.3						249
$\text{Li}_{6.62}\text{La}_3\text{Zr}_{1.62}\text{Nb}_{0.38}\text{O}_{12}$	4.41E-4	0.31						249
$\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.5}\text{Nb}_{0.5}\text{O}_{12}$	2.98E-4	0.319						249
$\text{Li}_6\text{La}_3\text{ZrNbO}_{12}$	1.50E-4	0.42						249
$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	3E-5	0.44						249
$\text{Li}_7\text{La}_3\text{Hf}_2\text{O}_{12}$	2.4E-4	0.29						250
Li_7GePS_8	7E-3	0.22						251
$\text{Li}_{10}(\text{Ge}_{0.95}\text{Si}_{0.05})\text{P}_2\text{S}_{12}$	8.63E-3	0.251						252
$\text{Li}_{10}(\text{Ge}_{0.9}\text{Si}_{0.1})\text{P}_2\text{S}_{12}$	8.07E-3	0.26						252
$\text{Li}_{10}(\text{Ge}_{0.8}\text{Si}_{0.2})\text{P}_2\text{S}_{12}$	7.28E-3	0.261						252
$\text{Li}_{10}(\text{Ge}_{0.7}\text{Si}_{0.3})\text{P}_2\text{S}_{12}$	5.82E-3	0.265						252
$\text{Li}_{10}(\text{Ge}_{0.6}\text{Si}_{0.4})\text{P}_2\text{S}_{12}$	5.24E-3	0.28						252
$\text{Li}_{10}(\text{Ge}_{0.5}\text{Si}_{0.5})\text{P}_2\text{S}_{12}$	4.2E-3	0.284						252
$\text{Li}_{10}(\text{Ge}_{0.2}\text{Si}_{0.8})\text{P}_2\text{S}_{12}$	4.81E-3	0.269						252

$\text{Li}_{10}(\text{Ge}_{0.95}\text{Sn}_{0.05})\text{P}_2\text{S}_{12}$	7.8E-3	0.254						252
$\text{Li}_{10}(\text{Ge}_{0.9}\text{Sn}_{0.1})\text{P}_2\text{S}_{12}$	7.53E-3	0.256						252
$\text{Li}_{10}(\text{Ge}_{0.8}\text{Sn}_{0.2})\text{P}_2\text{S}_{12}$	7.06E-3	0.252						252
$\text{Li}_{10}(\text{Ge}_{0.7}\text{Sn}_{0.3})\text{P}_2\text{S}_{12}$	6.49E-3	0.254						252
$\text{Li}_{10}(\text{Ge}_{0.5}\text{Sn}_{0.5})\text{P}_2\text{S}_{12}$	6.17E-3	0.249						252
$\text{Li}_{10}(\text{Ge}_{0.4}\text{Sn}_{0.6})\text{P}_2\text{S}_{12}$	5.76E-3	0.265						252
$\text{Li}_{10}(\text{Ge}_{0.3}\text{Sn}_{0.7})\text{P}_2\text{S}_{12}$	5.56E-3	0.261						252
$\text{Li}_{10}(\text{Ge}_{0.2}\text{Sn}_{0.8})\text{P}_2\text{S}_{12}$	4.77E-3	0.269						252
$0.5(\text{Li}_2\text{O}) * 0.5(\text{P}_2\text{O}_5)$	1.1E-9	0.71						253
$0.58(\text{Li}_2\text{O}) * 0.5(\text{P}_2\text{O}_5)$	2E-8	0.60						253
$0.6(\text{Li}_2\text{O}) * 0.5(\text{P}_2\text{O}_5)$	3E-8	0.61						253
$0.63(\text{Li}_2\text{O}) * 0.5(\text{P}_2\text{O}_5)$	1.3E-7	0.56						253
$0.66(\text{Li}_2\text{O}) * 0.5(\text{P}_2\text{O}_5)$	2.3E-7	0.55						253
$0.7(\text{Li}_2\text{O}) * 0.5(\text{P}_2\text{O}_5)$	3E-7	0.57						253
$0.2(\text{Li}_2\text{S}) 0.8(\text{GeS}_2)$	1.1E-7	0.52						253
$0.3(\text{Li}_2\text{S}) 0.7(\text{GeS}_2)$	9.3E-7	0.48						253
$0.4(\text{Li}_2\text{S}) 0.6(\text{GeS}_2)$	2.9E-6	0.42						253
$0.5(\text{Li}_2\text{S}) 0.5(\text{GeS}_2)$	3.3E-5	0.35						253
$0.6(\text{Li}_2\text{S}) 0.4(\text{GeS}_2)$	9.2E-5	0.32						253
$0.63(\text{Li}_2\text{S}) 0.37(\text{GeS}_2)$	1.5E-4	0.34						253
$0.66(\text{Li}_2\text{S}) 0.34(\text{GeS}_2)$	1.0E-4	0.37						253
$0.7(\text{Li}_2\text{S}) 0.3(\text{GeS}_2)$	1.2E-4	0.34						253
$\text{Li}_2\text{O-P}_2\text{O}_5$	1.1E-9	0.71						253
$0.58\text{Li}_2\text{O}-0.42\text{P}_2\text{O}_5$	2.0E-8	0.60						253
$0.6\text{Li}_2\text{O}-0.4\text{P}_2\text{O}_5$	3.0E-8	0.61						253

0.63Li ₂ O-0.37P ₂ O ₅	1.3E-7	0.56					253
0.66Li ₂ O-0.34P ₂ O ₅	2.3E-7	0.55					253
0.7Li ₂ O-0.3P ₂ O ₅	3.0E-7	0.57					253
0.2Li ₂ S-0.8GeS ₂	1.1E-7	0.52					253
0.3Li ₂ S-0.7GeS ₂	9.3E-7	0.48					253
0.4Li ₂ S-0.6GeS ₂	2.9E-6	0.42					253
0.5Li ₂ S-0.5GeS ₂	3.3E-5	0.35					253
0.6Li ₂ S-0.4GeS ₂	9.2E-5	0.32					253
0.63Li ₂ S-0.37GeS ₂	1.5E-4	0.34					253
0.66Li ₂ S-0.34GeS ₂	1.0E-4	0.37					253
0.7Li ₂ S-0.3GeS ₂	1.2E-4	0.34					253
Li _{6.55} La ₃ Zr ₂ Ga _{0.15} O ₁₂	1.3E-3	0.3					254
Li _{6.40} La ₃ Zr ₂ Ga _{0.2} O ₁₂	9E-4	0.3					254
Li _{6.10} La ₃ Zr ₂ Ga _{0.25} O ₁₂	7E-5	0.3					254
Li _{6.8} La ₃ Zr _{1.8} Sb _{0.2} O ₁₂	5.9E-5	0.39					255
Li _{6.6} La ₃ Zr _{1.6} Sb _{0.4} O ₁₂	7.7E-4	0.34					255
Li _{6.4} La ₃ Zr _{1.4} Sb _{0.6} O ₁₂	6.6E-4	0.36					255
Li _{6.2} La ₃ Zr _{1.2} Sb _{0.8} O ₁₂	4.5E-4	0.37					255
Li ₆ La ₃ ZrSbO ₁₂	2.6E-4	0.38					255
Li(Ind _{0.62} Li _{1.38})Br _{3.92}	4.9E-6	0.58					256
Li ₃ InBr ₆	1.77E-4						257
Li ₃ InBr ₄ Cl ₂	7.58E-6						257
Li ₃ InBr ₃ Cl ₃	1.14E-4						257
Li ₃ InBr _{2.5} Cl _{3.5}	3.60E-6						257
Li ₃ InBr ₂ Cl ₄	6.89E-8						257

$\text{Li}_{1.8}\text{Mg}_{1.1}\text{Cl}_4$	1.52E-6						258
$\text{Li}_{1.6}\text{Mg}_{1.2}\text{Cl}_4$	3.07E-6						258
$\text{Li}_{1.34}\text{Mg}_{1.33}\text{Cl}_4$	3.07E-6						258
$\text{Li}_{1.9}\text{Mn}_{1.05}\text{Cl}_4$	4.61E-6						258
$\text{Li}_{1.72}\text{Mn}_{1.14}\text{Cl}_4$	3.62E-6						258
$\text{Li}_{1.6}\text{Mn}_{1.2}\text{Cl}_4$	1.45E-5						258
$\text{Li}_{1.52}\text{Mn}_{1.24}\text{Cl}_4$	1.85E-5						258
$\text{Li}_{1.34}\text{Mn}_{1.33}\text{Cl}_4$	9.57E-6						258
$\text{Li}_{1.94}\text{Cl}_{1.03}\text{Cl}_4$	2.56E-6						258
$\text{Li}_{1.90}\text{Cd}_{1.05}\text{Cl}_4$	3.50E-6						258
Li_2OHBrF	7.10E-7						259
$\text{Li}_2\text{OHBr}_{0.99}\text{F}_{0.01}$	9.16E-7						259
$\text{Li}_2\text{OHBr}_{0.98}\text{F}_{0.02}$	1.11E-6						259
$\text{Li}_2\text{OHBr}_{0.95}\text{F}_{0.05}$	6.75E-7						259
$\text{Li}_2\text{OHBr}_{0.9}\text{F}_{0.1}$	6.80E-7						259
$\text{Li}_2\text{OHBr}_{0.8}\text{F}_{0.2}$	5.44E-7						259
$\text{Li}_3(\text{OH})_2\text{Cl}$	2.72E-8	0.88					260
$\text{Li}_5(\text{OH})_3\text{Cl}_2$	2.52E-8	0.75					260
Li_2OHCl	4.28E-8	0.56					260
$\text{Li}_5(\text{OH})_2\text{Cl}_3$	1.48E-7	0.49					260
Li_3OHCl_2	8.92E-8	0.67					260
$\text{Li}_{3.7}\text{Zn}_{0.15}\text{GeO}_4$	4.63E-7						261
$\text{Li}_{3.5}\text{Zn}_{0.25}\text{GeO}_4$	2.42E-7						261
$\text{Li}_{3.1}\text{Zn}_{0.45}\text{GeO}_4$	9.89E-8						261
$\text{Li}_{2.8}\text{Zn}_{0.6}\text{GeO}_4$	1.27E-7						261

$\text{Li}_{2.6}\text{Zn}_{0.7}\text{GeO}_4$	5.79E-8						261
$\text{Li}_{2.3}\text{Zn}_{0.85}\text{GeO}_4$	4.23E-9						261
$\text{Li}_7\text{La}_{2.75}\text{Ca}_{0.25}\text{Zr}_{1.75}\text{Nb}_{0.2}\text{O}_{12}$	2.2E-4	0.35					262
$\text{Li}_{1.5}\text{Cr}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	1.98E-4	0.29					263
$\text{Li}_3\text{V}_2(\text{PO}_4)_3$	2.09E-7						263
$\text{Li}_3\text{V}_{1.8}\text{Al}_{0.2}(\text{PO}_4)_3$	1.88E-6						263
$\text{Li}_3\text{V}_{1.6}\text{Al}_{0.4}(\text{PO}_4)_3$	6.21E-6						263
$\text{Li}_3\text{V}_{1.4}\text{Al}_{0.6}(\text{PO}_4)_3$	9.34E-7						263
$\text{Li}_7\text{P}_{2.9}\text{Mn}_{0.1}\text{S}_{10.7}\text{l}_{0.3}$	5.6E-3	0.22					264
0.3 Li_2S * 0.7 SiS_2	1.6E-6	0.46					265
0.4 Li_2S * 0.6 SiS_2	2.8E-5	0.38					265
0.5 Li_2S * 0.5 SiS_2	1.0E-4	0.32					265
0.6 Li_2S * 0.4 SiS_2	5.0E-4	0.25					265
(2 Li_2S - P_2S_5)	1.12E-4						266
(2 Li_2S - P_2S_5) _{0.85} (LiI) _{0.15}	2.35E-4						266
(2 Li_2S - P_2S_5) _{0.75} (LiI) _{0.25}	3.96E-4						266
(2 Li_2S - P_2S_5) _{0.60} (LiI) _{0.40}	7.60E-4						266
(2 Li_2S - P_2S_5) _{0.55} (LiI) _{0.45}	1.12E-3						266
0.14 SiS_2 -0.09 P_2S_5 - 0.47 Li_2S -0.30 LiI	1.32E-3	0.34					267
0.26 B_2S_3 - 0.3 Li_2S - 0.44 LiI	1.57E-3	0.3					268
0.26 B_2S_3 - 0.31 Li_2S - 0.43 LiI	7.99E-4	0.33					268
0.27 B_2S_3 - 0.32 Li_2S - 0.41 LiI	4.25E-4	0.35					268
0.5 SiS_2 -0.5 Li_2S	1.5E-4	0.34					269

0.1 LiBr-0.45 SiS ₂ -0.45 Li ₂ S	1.9E-4	0.30					269
0.2 LiBr-0.4 SiS ₂ -0.4 Li ₂ S	2.1E-4	0.33					269
0.25 LiBr-0.38 SiS ₂ -0.38 Li ₂ S	2.4E-4	0.31					269
0.3 LiBr-0.3 SiS ₂ -0.35 Li ₂ S	3.2E-4	0.33					269
0.35 LiBr-0.33 SiS ₂ -0.33 Li ₂ S	2.3E-4	0.38					269
0.4 LiBr-0.3 SiS ₂ -0.3 Li ₂ S	1.1E-4	0.42					269
SiS ₂ -Li ₂ S	1.20E-4	0.35					270
0.9(SiS ₂ -Li ₂ S)-0.1LiCl	1.84E-4	0.34					270
0.8(SiS ₂ -Li ₂ S)-0.2LiCl	2.35E-4	0.33					270
0.75(SiS ₂ -Li ₂ S)-0.25LiCl	2.66E-4	0.35					270
0.7(SiS ₂ -Li ₂ S)-0.3LiCl	2.33E-4	0.35					270
0.65(SiS ₂ -Li ₂ S)-0.35LiCl	1.78E-4	0.36					270
0.6(SiS ₂ -Li ₂ S)-0.4LiCl	0.93E-4	0.34					270
(0.4SiS ₂ -0.6Li ₂ S)	5.3E-4	0.33					271
0.9(0.4SiS ₂ -0.6Li ₂ S)-0.1LiI	6.5E-4	0.31					271
0.8(0.4SiS ₂ -0.6Li ₂ S)-0.2LiI	7.7E-4	0.30					271
0.7(0.4SiS ₂ -0.6Li ₂ S)-0.3LiI	1.15E-3	0.29					271
0.6(0.4SiS ₂ -0.6Li ₂ S)-0.4LiI	1.78E-3	0.28					271
0.55(0.4SiS ₂ -0.6Li ₂ S)-0.45LiI	1.41E-3	0.29					271

0.24SiS ₂ -0.36Li ₂ S-0.4LiI	1.8E-3	0.28					272
0.28SiS ₂ -0.42Li ₂ S-0.30LiI	1.8E-3	0.31					273
0.14SiS ₂ -0.09P ₂ S ₅ -0.47Li ₂ S-0.30LiI	2.1E-3	0.34					273
0.27SiS ₂ -0.03Al ₂ S ₃ -0.30Li ₂ S-0.40LiI	1.2E-3	0.34					273
0.21SiS ₂ -0.09B ₂ S ₃ -0.30Li ₂ S-0.40LiI	1.7E-3	0.30					273
0.30Li ₂ S-0.7GeS ₂	4.4E-7	0.63					274
0.40Li ₂ S-0.60GeS ₂	3.2E-6	0.52					274
0.50Li ₂ S-0.50GeS ₂	4.0E-5	0.51					274
0.3Li ₂ S-0.7P ₂ S ₅	1.7E-2	0.18					275
0.7Li ₂ S-0.3P ₂ S ₅	3.2E-3	0.12					276
0.6Li ₂ S-0.4P ₂ S ₅	1.5E-4	0.31					277
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₄ SiO ₄	1.58E-3	0.34					278
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₄ SiO ₄	4.34E-4	0.37					278
0.8(0.6Li ₂ S-0.4SiS ₂)-0.2Li ₄ SiO ₄	1.59E-4	0.43					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ PO ₄	8.68E-4	0.35					278
0.7(0.6Li ₂ S-0.4SiS ₂)-0.3Li ₃ PO ₄	2.08E-5	0.46					278
0.6(0.6Li ₂ S-0.4SiS ₂)-0.4Li ₃ PO ₄	5.33E-6	0.51					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₄ GeO ₄	1.19E-3	0.28					278
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₄ GeO ₄	3.18E-4	0.35					278

0.85(0.6Li ₂ S-0.4SiS ₂)-0.15Li ₄ GeO ₄	1.14E-4	0.40					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ BO ₃	1.44E-3	0.33					278
0.93(0.6Li ₂ S-0.4SiS ₂)-0.07Li ₃ BO ₃	3.84E-4	0.35					278
0.85(0.6Li ₂ S-0.4SiS ₂)-0.15Li ₃ BO ₃	3.42E-4	0.36					278
0.75(0.6Li ₂ S-0.4SiS ₂)-0.25Li ₃ BO ₃	7.06E-5	0.38					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ AlO ₃	1.31E-3	0.31					278
0.94(0.6Li ₂ S-0.4SiS ₂)-0.06Li ₃ AlO ₃	6.83E-4	0.34					278
0.92(0.6Li ₂ S-0.4SiS ₂)-0.08Li ₃ AlO ₃	4.04E-4	0.34					278
0.825(0.6Li ₂ S-0.4SiS ₂)-0.175Li ₃ AlO ₃	1.31E-4	0.36					278
0.975(0.6Li ₂ S-0.4SiS ₂)-0.025Li ₃ GaO ₃	6.82E-4	0.31					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ GaO ₃	3.25E-4	0.32					278
0.92(0.6Li ₂ S-0.4SiS ₂)-0.08Li ₃ GaO ₃	3.03E-4	0.35					278
0.89(0.6Li ₂ S-0.4SiS ₂)-0.11Li ₃ GaO ₃	1.13E-4	0.38					278
0.97(0.6Li ₂ S-0.4SiS ₂)-0.03Li ₃ InO ₃	3.09E-4	0.34					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ InO ₃	3.25E-4	0.35					278
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₃ InO ₃	6.84E-5	0.40					278
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₄ SiO ₄	1.54E-3	0.38					279

0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₄ SiO ₄	4.39E-4	0.40					279
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₂ SO ₄	4.53E-4	0.41					279
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₂ SO ₄	4.70E-5	0.45					279
0.5Li ₂ O-0.1TiO ₂ -0.4P ₂ O ₅	5.67E-8	0.56					280
0.5025Li ₂ O-0.0025Al ₂ O ₃ -0.095TiO ₂ -0.4P ₂ O ₅	1.56E-8	0.55					280
0.505Li ₂ O-0.005Al ₂ O ₃ -0.09TiO ₂ -0.4P ₂ O ₅	1.78E-7	0.50					280
0.5075Li ₂ O-0.0075Al ₂ O ₃ -0.085TiO ₂ -0.4P ₂ O ₅	2.51E-7	0.57					280
0.51Li ₂ O-0.01Al ₂ O ₃ -0.08TiO ₂ -0.4P ₂ O ₅	1.58E-7	0.55					280
0.515Li ₂ O-0.015Al ₂ O ₃ -0.07TiO ₂ -0.4P ₂ O ₅	1.25E-7	0.56					280
0.525Li ₂ O-0.025Al ₂ O ₃ -0.05TiO ₂ -0.4P ₂ O ₅	2.17E-7	0.56					280
0.53Li ₂ O-0.03Al ₂ O ₃ -0.04TiO ₂ -0.4P ₂ O ₅	2.72E-7	0.54					280
0.54Li ₂ O-0.04Al ₂ O ₃ -0.02TiO ₂ -0.4P ₂ O ₅	1.97E-7	0.55					280
0.545Li ₂ O-0.045Al ₂ O ₃ -0.01TiO ₂ -0.4P ₂ O ₅	7.14E-8	0.56					280
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₄ SiO ₄	1.51E-3	0.34					281
0.90(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₄ SiO ₄	4.34E-4	0.37					281
0.8(0.6Li ₂ S-0.4SiS ₂)-0.2Li ₄ SiO ₄	1.63E-4	0.43					281

0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ PO ₄	9.32E-4	0.35					281
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₃ PO ₄	4.55E-4	0.37					281
0.7(0.6Li ₂ S-0.4SiS ₂)-0.3Li ₃ PO ₄	2.08E-5	0.46					281
0.6(0.6Li ₂ S-0.4SiS ₂)-0.4Li ₃ PO ₄	5.33E-6	0.51					281
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₄ GeO ₄	1.21E-3	0.28					281
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₄ GeO ₄	3.18E-4	0.34					281
0.85(0.6Li ₂ S-0.4SiS ₂)-0.15Li ₄ GeO ₄	1.14E-4	0.41					281
Li ₇ PS ₆	8.0E-5						282
0.7Li ₂ S-0.3P ₂ S ₅	3.2E-3	0.12					283
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ BO ₃	1.40E-3						284
0.93(0.6Li ₂ S-0.4SiS ₂)-0.07Li ₃ BO ₃	3.71E-4						284
0.85(0.6Li ₂ S-0.4SiS ₂)-0.15Li ₃ BO ₃	3.39E-4						284
0.75(0.6Li ₂ S-0.4SiS ₂)-0.25Li ₃ BO ₃	7.15E-5						284
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ AlO ₃	1.22E-3						284
0.94(0.6Li ₂ S-0.4SiS ₂)-0.06Li ₃ AlO ₃	6.67E-4						284
0.92(0.6Li ₂ S-0.4SiS ₂)-0.08Li ₃ AlO ₃	3.94E-4						284
0.825(0.6Li ₂ S-0.4SiS ₂)-0.175Li ₃ AlO ₃	1.25E-4						284

0.975(0.6Li ₂ S-0.4SiS ₂)- 0.025Li ₃ GaO ₃	7.05E-4						284
0.95(0.6Li ₂ S-0.4SiS ₂)- 0.05Li ₃ GaO ₃	3.36E-4						284
0.92(0.6Li ₂ S-0.4SiS ₂)- 0.08Li ₃ GaO ₃	3.06E-4						284
0.89(0.6Li ₂ S-0.4SiS ₂)- 0.11Li ₃ GaO ₃	1.20E-4						284
0.97(0.6Li ₂ S-0.4SiS ₂)- 0.03Li ₃ InO ₃	3.11E-4						284
0.95(0.6Li ₂ S-0.4SiS ₂)- 0.05Li ₃ InO ₃	2.99E-4						284
0.90(0.6Li ₂ S-0.4SiS ₂)- 0.10Li ₃ InO ₃	6.81E-5						284
(0.67Li ₂ S-0.33SiS ₂)- (0.75Li ₂ S-0.25P ₂ S ₅)	1.2E-3	0.28					285
0.2Li ₃ N-0.8SiS ₂	1.46E-6	0.45					286
0.3Li ₃ N-0.7SiS ₂	2.97E-5	0.36					286
0.4Li ₃ N-0.6SiS ₂	2.74E-4	0.30					286
0.5Li ₃ N-0.5SiS ₂	4.47E-5	0.34					286
0.6Li ₃ N-0.4SiS ₂	2.25E-8	0.63					286
0.6Li ₂ S-0.4P ₂ S ₃	5.70E-6						287
0.63Li ₂ S-0.37P ₂ S ₃	2.55E-5						287
0.667Li ₂ S-0.333P ₂ S ₃	1.1E-4	0.40					287
0.7Li ₂ S-0.3P ₂ S ₃	7.90E-5						287
0.75Li ₂ S-0.25P ₂ S ₃	5.08E-5						287
0.6Li ₂ S-0.4SiS ₂	5.1E-4	0.33					288
0.555Li ₂ S-0.4SiS ₂ - 0.045Li ₃ N	1.5E-3	0.28					288

0.525Li ₂ S-0.4SiS ₂ -0.075Li ₃ N	9.6E-4	0.29					288
0.1Li ₂ O-0.1LiCl-0.65B ₂ O ₃ -0.1SiO ₂ -0.05Al ₂ O ₃	1.9E-4	0.427					289
0.75Li ₂ O-0.25P ₂ S ₅	1.80E-5	0.48					290
0.75(0.7Li ₂ O-0.3Li ₂ S)-0.25P ₂ S ₅	2.42E-5	0.48					290
0.75(0.5Li ₂ O-0.5Li ₂ S)-0.25P ₂ S ₅	2.83E-5	0.46					290
0.75(0.4Li ₂ O-0.6Li ₂ S)-0.25P ₂ S ₅	4.99E-5	0.44					290
0.75(0.3Li ₂ O-0.7Li ₂ S)-0.25P ₂ S ₅	8.89E-5	0.40					290
0.75(0.2Li ₂ O-0.8Li ₂ S)-0.25P ₂ S ₅	1.63E-4	0.38					290
0.75(0.1Li ₂ O-0.9Li ₂ S)-0.25P ₂ S ₅	2.27E-4	0.36					290
0.75Li ₂ S-0.25P ₂ S ₅	1.80E-4	0.41					290
0.45Li ₂ -0.55SiS ₂	1.08E-4	0.40					291
0.5Li ₂ -0.5SiS ₂	3.36E-4	0.32					291
0.55Li ₂ -0.45SiS ₂	6.53E-4	0.30					291
0.60Li ₂ -0.4SiS ₂	1.19E-3	0.29					291
0.63Li ₂ -0.37SiS ₂	1.05E-3	0.30					291
0.65Li ₂ -0.35SiS ₂	7.41E-4	0.33					291
0.95(0.5Li ₂ -0.5SiS ₂)-0.05(0.5Li ₂ O-0.5P ₂ O ₅)	4.27E-4	0.38					291
0.95(0.53Li ₂ -0.47SiS ₂)-0.05(0.53Li ₂ O-0.47P ₂ O ₅)	5.91E-4	0.33					291

0.95(0.55Li ₂ -0.45SiS ₂)- 0.05(0.55Li ₂ O- 0.45P ₂ O ₅)	1.01E-3	0.34					291
0.95(0.58Li ₂ -0.42SiS ₂)- 0.05(0.58Li ₂ O- 0.42P ₂ O ₅)	1.06E-3	0.34					291
0.95(0.6Li ₂ -0.4SiS ₂)- 0.05(0.6Li ₂ O-0.4P ₂ O ₅)	1.01E-3	0.27					291
0.95(0.63Li ₂ -0.37SiS ₂)- 0.05(0.63Li ₂ O- 0.37P ₂ O ₅)	8.71E-4	0.33					291
0.95(0.65Li ₂ -0.35SiS ₂)- 0.05(0.65Li ₂ O- 0.35P ₂ O ₅)	5.34E-4	0.32					291
0.95(0.67Li ₂ -0.33SiS ₂)- 0.05(0.67Li ₂ O- 0.33P ₂ O ₅)	1.99E-4	0.37					291
0.8(0.55Li ₂ -0.45SiS ₂)- 0.2(0.55Li ₂ O-0.45P ₂ O ₅)	7.88E-5	0.41					291
0.8(0.6Li ₂ -0.4SiS ₂)- 0.2(0.6Li ₂ O-0.4P ₂ O ₅)	7.69E-5	0.41					291
0.8(0.65Li ₂ -0.35SiS ₂)- 0.2(0.65Li ₂ O-0.35P ₂ O ₅)	5.21E-5	0.42					291
0.65Li ₂ S-0.35P ₂ S ₅	4.14E-5						292
0.675Li ₂ S-0.325P ₂ S ₅	7.84E-5						292
0.7Li ₂ S-0.3P ₂ S ₅	1.58E-3	0.39					292
0.725Li ₂ S-0.275P ₂ S ₅	4.51E-4						292
0.75Li ₂ S-0.25P ₂ S ₅	3.67E-4						292
0.6Li ₂ S-0.4SiS ₂	1.69E-4						293
0.1LiI-0.9(0.6Li ₂ S- 0.4SiS ₂)	2.35E-4						293
0.2LiI-0.8(0.6Li ₂ S- 0.4SiS ₂)	3.52E-4						293

0.3LiI-0.7(0.6Li ₂ S-0.4SiS ₂)	7.42E-4						293
0.5Li ₂ S-0.5SiS ₂	1.58E-6						293
0.1LiI-0.9(0.5Li ₂ S-0.5SiS ₂)	3.99E-5						293
0.2LiI-0.8(0.6Li ₂ S-0.4SiS ₂)	1.23E-4						293
0.3LiI-0.7(0.6Li ₂ S-0.4SiS ₂)	3.62E-4						293
Li ₆ Si ₂ S ₇	4.11E-4	0.37					294
0.95Li ₆ Si ₂ S ₇ -0.05Li ₆ B ₄ O ₉	4.11E-4	0.35					294
0.9Li ₆ Si ₂ S ₇ -0.1Li ₆ B ₄ O ₉	3.76E-4	0.39					294
0.875Li ₆ Si ₂ S ₇ -0.125Li ₆ B ₄ O ₉	2.77E-4	0.39					294
0.75Li ₆ Si ₂ S ₇ -0.25Li ₆ B ₄ O ₉	1.42E-4	0.40					294
0.95Li ₆ Si ₂ S ₇ -0.05Li ₆ B ₄ S ₉	4.90E-4	0.37					294
0.925Li ₆ Si ₂ S ₇ -0.075Li ₆ B ₄ S ₉	3.65E-4	0.38					294
0.9Li ₆ Si ₂ S ₇ -0.1Li ₆ B ₄ S ₉	4.73E-4	0.38					294
0.875Li ₆ Si ₂ S ₇ -0.125Li ₆ B ₄ S ₉	4.40E-4	0.37					294
0.75Li ₆ Si ₂ S ₇ -0.25Li ₆ B ₄ S ₉	5.02E-4	0.36					294
0.63Li ₆ Si ₂ S ₇ -0.37Li ₆ B ₄ S ₉	4.39E-4	0.39					294
(Li ₂ S) ₆₀ (SiS ₂) ₂₈ (P ₂ S ₅) ₁₂	1.23E-3	0.34					295
Li ₇ La ₃ Zr ₂ O ₁₂ -5 wt% LiPO ₃	2.5E-6	0.51					120

Li ₇ La ₃ Zr ₂ O ₁₂ -3 wt% 65Li ₂ O·27B ₂ O ₃ ·8SiO ₂	1.5E-5	0.44					120
Li ₇ La ₃ Zr ₂ O ₁₂ -5 wt% 40.2Li ₂ O·5.7Y ₂ O ₃ ·54.1 SiO ₂	2.5E-5	0.39					120
0.6Li ₂ S-0.4P ₂ S ₅	3.32E-6	0.52					296
0.667Li ₂ S-0.333P ₂ S ₅	3.836E-5	0.44					296
0.7Li ₂ S-0.3P ₂ S ₅	3.77E-5	0.45					296
0.75Li ₂ S-0.25P ₂ S ₅	2.79E-4	0.40					296
0.8Li ₂ S-0.2P ₂ S ₅	1.32E-4	0.44					296
(0.75Li ₂ S-0.25P ₂ S ₅)	2.68E-4	0.26					297
0.95(0.75Li ₂ S- 0.25P ₂ S ₅)-0.05LiBH ₄	3.98E-4	0.25					297
0.89(0.75Li ₂ S- 0.25P ₂ S ₅)-0.11LiBH ₄	6.18E-4	0.26					297
0.67(0.75Li ₂ S- 0.25P ₂ S ₅)-0.33LiBH ₄	1.13E-3	0.21					297
Li ₇ P _{2.9} S _{10.85} Mo _{0.01}	4.8E-3	0.24					298
Li ₇ P ₃ S ₁₁	2.6E-3	0.29					298
Li ₇ P _{2.9} Mn _{0.1} S _{10.7} I _{0.3}	5.6E-3	0.22					299
Li ₁₁ AlP ₂ S ₁₂	8.02E-4	0.26					300
Li ₃ PS ₄	1.78E-4	0.33					301
Li ₃ PS ₄ - 2 wt% Al ₂ O ₃	2.27E-4	0.35					301
Li ₃ PS ₄ - 5 wt% Al ₂ O ₃	1.96E-4	0.35					301
Li ₃ PS ₄ - 8 wt% Al ₂ O ₃	1.60E-4	0.36					301
Li ₃ PS ₄ - 10 wt% Al ₂ O ₃	1.50E-4	0.36					301
Li ₃ PS ₄ - 30 wt% Al ₂ O ₃	9.96E-5	0.36					301
Li ₃ PS ₄ - 50 wt% Al ₂ O ₃	9.38E-7	0.44					301

Li_3PS_4 – 70 wt% Al_2O_3	3.92E-8	0.60					301
Li_3PS_4 – 90 wt% Al_2O_3	1.54E-9	0.79					301
Li_3PS_4 – 2 wt% SiO_2	2.28E-4	0.32					301
Li_3PS_4 – 5 wt% SiO_2	1.96E-4	0.33					301
Li_3PS_4 – 8 wt% SiO_2	1.60E-4	0.33					301
Li_3PS_4 – 10 wt% SiO_2	1.50E-4	0.33					301
Li_3PS_4 – 30 wt% SiO_2	1.00E-4	0.35					301
Li_3PS_4 – 50 wt% SiO_2	3.80E-5	0.36					301
Li_3PS_4 – 70 wt% SiO_2	5.92E-6	0.38					301
Li_3PS_4 – 90 wt% SiO_2	8.53E-9	0.41					301
Li_3PS_4 – 5 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	2.28E-4	0.29					301
Li_3PS_4 – 10 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	2.43E-4	0.31					301
Li_3PS_4 – 15 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	2.41E-4	0.32					301
Li_3PS_4 – 20 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	2.22E-4	0.33					301
Li_3PS_4 – 30 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	1.87E-4	0.34					301
Li_3PS_4 – 50 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	1.42E-4	0.36					301
Li_3PS_4 – 70 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	7.23E-5	0.38					301
Li_3PS_4 – 90 wt% $\text{Li}_6\text{ZnNb}_4\text{O}_{14}$	2.99E-7	0.40					301
Li_3PS_4	1.46E-4	0.38					302
Li_3PS_4 – 10 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	2.96E-4	0.36					302

Li_3PS_4 -20 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	3.70E-4	0.35					302
Li_3PS_4 -25 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	4.10E-4	0.35					302
Li_3PS_4 -30 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	5.38E-4	0.36					302
Li_3PS_4 -35 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	4.00E-4	0.36					302
Li_3PS_4 -40 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	3.33E-4	0.36					302
Li_3PS_4 -60 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	2.19E-4	0.40					302
Li_3PS_4 -70 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.26E-5	0.43					302
Li_3PS_4 -90 wt% $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	6.04E-6	0.44					302
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	5.20E-8	0.47					302
$\text{Li}_{3.45}\text{Ge}_{0.45}\text{P}_{0.55}\text{S}_{3.1}\text{Se}_{0.9}$	9.8E-4						303
$\text{Li}_{3.4}\text{Ge}_{0.4}\text{P}_{0.6}\text{S}_{3.2}\text{Se}_{0.8}$	1.17E-3						303
$\text{Li}_{3.35}\text{Ge}_{0.35}\text{P}_{0.65}\text{S}_{3.3}\text{Se}_{0.7}$	1.20E-3						303
$\text{Li}_{3.3}\text{Ge}_{0.3}\text{P}_{0.7}\text{S}_{3.4}\text{Se}_{0.6}$	1.33E-3						303
$\text{Li}_{3.25}\text{Ge}_{0.25}\text{P}_{0.75}\text{S}_{3.5}\text{Se}_{0.5}$	5.03E-4						303
$\text{Li}_{3.20}\text{Ge}_{0.20}\text{P}_{0.8}\text{S}_{3.6}\text{Se}_{0.4}$	1.08E-3						303
$\text{Li}_{3.15}\text{Ge}_{0.15}\text{P}_{0.85}\text{S}_{3.7}\text{Se}_{0.3}$	8.16E-4						303
$\text{Li}_{3.1}\text{Ge}_{0.1}\text{P}_{0.9}\text{S}_{3.8}\text{Se}_{0.2}$	1.13E-3						303
$\text{Li}_{3.05}\text{Ge}_{0.05}\text{P}_{0.95}\text{S}_{3.9}\text{Se}_{0.1}$	1.41E-3						303
Li_3PS_4	9.35E-4						303
$0.8\text{Li}_2\text{O}-0.2\text{P}_2\text{S}_5$	1.54E-5						304
$0.05\text{Li}_2\text{S}-0.75\text{Li}_2\text{O}-0.2\text{P}_2\text{S}_5$	1.39E-5						304

0.1Li ₂ S-0.7Li ₂ O-0.2P ₂ S ₅	1.59E-5						304
0.15Li ₂ S-0.65Li ₂ O-0.2P ₂ S ₅	2.32E-5						304
0.2Li ₂ S-0.6Li ₂ O-0.2P ₂ S ₅	2.89E-5						304
0.25Li ₂ S-0.55Li ₂ O-0.2P ₂ S ₅	3.80E-5						304
0.3Li ₂ S-0.5Li ₂ O-0.2P ₂ S ₅	4.35E-5						304
0.35Li ₂ S-0.45Li ₂ O-0.2P ₂ S ₅	5.26E-5						304
0.4Li ₂ S-0.4Li ₂ O-0.2P ₂ S ₅	4.45E-5						304
0.45Li ₂ S-0.35Li ₂ O-0.2P ₂ S ₅	6.35E-5						304
0.5Li ₂ S-0.3Li ₂ O-0.2P ₂ S ₅	8.11E-5						304
0.55Li ₂ S-0.25Li ₂ O-0.2P ₂ S ₅	1.12E-4						304
0.6Li ₂ S-0.2Li ₂ O-0.2P ₂ S ₅	1.12E-4						304
0.65Li ₂ S-0.15Li ₂ O-0.2P ₂ S ₅	1.13E-4						304
0.7Li ₂ S-0.1Li ₂ O-0.2P ₂ S ₅	1.09E-4						304
0.75Li ₂ S-0.05Li ₂ O-0.2P ₂ S ₅	1.43E-4						304
0.8Li ₂ S-0.2P ₂ S ₅	2.99E-4						304
0.75Li ₂ O-0.25P ₂ S ₅	1.55E-5						304
0.05Li ₂ S-0.7Li ₂ O-0.25P ₂ S ₅	1.42E-5						304

0.1Li ₂ S-0.65Li ₂ O-0.25P ₂ S ₅	2.52E-5						304
0.15Li ₂ S-0.6Li ₂ O-0.25P ₂ S ₅	2.67E-5						304
0.2Li ₂ S-0.55Li ₂ O-0.25P ₂ S ₅	2.74E-5						304
0.25Li ₂ S-0.5Li ₂ O-0.25P ₂ S ₅	3.80E-5						304
0.3Li ₂ S-0.45Li ₂ O-0.25P ₂ S ₅	5.88E-5						304
0.35Li ₂ S-0.4Li ₂ O-0.25P ₂ S ₅	1.33E-5						304
0.4Li ₂ S-0.35Li ₂ O-0.25P ₂ S ₅	2.44E-5						304
0.45Li ₂ S-0.3Li ₂ O-0.25P ₂ S ₅	2.30E-5						304
0.5Li ₂ S-0.25Li ₂ O-0.25P ₂ S ₅	9.56E-6						304
0.55Li ₂ S-0.2Li ₂ O-0.25P ₂ S ₅	7.06E-5						304
0.6Li ₂ S-0.15Li ₂ O-0.25P ₂ S ₅	9.27E-5						304
0.65Li ₂ S-0.1Li ₂ O-0.25P ₂ S ₅	1.15E-4						304
0.7Li ₂ S-0.05Li ₂ O-0.25P ₂ S ₅	9.76E-5						304
0.75Li ₂ S-0.25P ₂ S ₅	1.60E-4						304
0.7Li ₂ O-0.3P ₂ S ₅	5.78E-11						304
0.05Li ₂ S-0.65Li ₂ O-0.3P ₂ S ₅	1.51E-8						304
0.1Li ₂ S-0.6Li ₂ O-0.3P ₂ S ₅	7.78E-8						304

0.15Li ₂ S-0.55Li ₂ O-0.3P ₂ S ₅	2.90E-7						304
0.2Li ₂ S-0.5Li ₂ O-0.3P ₂ S ₅	1.67E-5						304
0.25Li ₂ S-0.45Li ₂ O-0.3P ₂ S ₅	8.64E-7						304
0.3Li ₂ S-0.4Li ₂ O-0.3P ₂ S ₅	1.62E-6						304
0.35Li ₂ S-0.35Li ₂ O-0.3P ₂ S ₅	3.68E-6						304
0.4Li ₂ S-0.3Li ₂ O-0.3P ₂ S ₅	5.86E-6						304
0.45Li ₂ S-0.25Li ₂ O-0.3P ₂ S ₅	5.10E-6						304
0.5Li ₂ S-0.2Li ₂ O-0.3P ₂ S ₅	8.33E-6						304
0.55Li ₂ S-0.15Li ₂ O-0.3P ₂ S ₅	1.01E-5						304
0.6Li ₂ S-0.1Li ₂ O-0.3P ₂ S ₅	2.29E-5						304
0.65Li ₂ S-0.05Li ₂ O-0.3P ₂ S ₅	2.48E-5						304
0.7Li ₂ S- 0.3P ₂ S ₅	5.34E-5						304
0.9Li ₃ PS ₄ ·10ZnO	2.9E-4						305
0.7Li ₂ S-0.3P ₂ S ₅	7.10E-4	0.23					306
0.7Li ₂ S-0.29P ₂ S ₅ -0.01Li ₃ PO ₄	1.83E-3	0.19					306
0.7Li ₂ S-0.28P ₂ S ₅ -0.02Li ₃ PO ₄	9.89E-4	0.21					306
0.7Li ₂ S-0.27P ₂ S ₅ -0.03Li ₃ PO ₄	4.40E-4	0.25					306
0.7Li ₂ S-0.25P ₂ S ₅ -0.05Li ₃ PO ₄	2.67E-4	0.29					306

0.7Li ₂ S-0.3P ₂ S ₅	1.67E-3	0.23					307
0.99(0.7Li ₂ S-0.3P ₂ S ₅)-0.01Li ₂ ZrO ₃	2.86E-3	0.18					307
0.98(0.7Li ₂ S-0.3P ₂ S ₅)-0.02Li ₂ ZrO ₃	1.22E-3	0.25					307
0.95(0.7Li ₂ S-0.3P ₂ S ₅)-0.05Li ₂ ZrO ₃	7.42E-4	0.29					307
Li _{2.7} PO _{3.9}	7E-8	0.68					308
Li _{3.6} (Si _{0.19} P _{0.82})O _{4.2}	2.0E-7	0.57					308
Li _{3.1} PO _{3.8} N _{0.16}	2.00E-6	0.57					308
Li _{3.3} PO _{3.8} N _{0.22}	2.40E-6	0.56					308
Li _{2.9} PO _{3.3} N _{0.46}	3.30E-6	0.54					308
Li _{4.4} PO _{4.3}	9.39E-7	0.64					309
Li _{4.0} PO _{3.9} N _{0.4}	1.70E-6	0.62					309
Li _{3.7} PO _{3.4} N _{0.7}	2.36E-6	0.60					309
Li _{3.5} PO _{3.2} N _{0.8}	2.59E-6	0.59					309
Li _{3.4} PO _{3.1} N _{0.9}	2.81E-6	0.58					309
Li _{3.2} PO _{3.0} N	2.99E-6	0.57					309
Li _{2.9} PO _{2.6} N _{0.91}	2.1E-6	0.52					310
Li _{1.8} PO _{1.2} N _{1.5}	1.7E-6	0.49					310
Li _{3.3} PO _{2.9} N _{0.83}	3.1E-6	0.47					310
0.45B ₂ S ₃ -0.55Li ₂ S	8.19E-5	0.23					311
0.815(0.45B ₂ S ₃ -0.55Li ₂ S)-0.185Lil	3.08E-4	0.20					311
0.69(0.45B ₂ S ₃ -0.55Li ₂ S)-0.31Lil	7.58E-4	0.23					311
0.33B ₂ S ₃ -0.67Li ₂ S	2.26E-4	0.31					311

0.95(0.33B ₂ S ₃ -0.67Li ₂ S)-0.05Lil	4.37E-4	0.29					311
0.9(0.33B ₂ S ₃ -0.67Li ₂ S)-0.1Lil	4.81E-4	0.28					311
0.85(0.33B ₂ S ₃ -0.67Li ₂ S)-0.15Lil	4.92E-4	0.28					311
0.75(0.33B ₂ S ₃ -0.67Li ₂ S)-0.25Lil	6.10E-4	0.27					311
0.66(0.33B ₂ S ₃ -0.67Li ₂ S)-0.34Lil	5.22E-4	0.32					311
0.6(0.33B ₂ S ₃ -0.67Li ₂ S)-0.4Lil	4.89E-4	0.35					311
0.29B ₂ S ₃ -0.71Li ₂ S	2.71E-4	0.32					311
0.95(0.29B ₂ S ₃ -0.71Li ₂ S)-0.05Lil	3.72E-4	0.31					311
0.875(0.29B ₂ S ₃ -0.71Li ₂ S)-0.125Lil	6.27E-4	0.29					311
0.78(0.29B ₂ S ₃ -0.71Li ₂ S)-0.22Lil	6.56E-4	0.29					311
0.64(0.29B ₂ S ₃ -0.71Li ₂ S)-0.36Lil	8.10E-4	0.36					311
0.25B ₂ S ₃ -0.75Li ₂ S	3.03E-4	0.36					311
0.92(0.25B ₂ S ₃ -0.75Li ₂ S)-0.08Lil	3.83E-4	0.30					311
0.89(0.25B ₂ S ₃ -0.75Li ₂ S)-0.11Lil	3.48E-4	0.33					311
0.5Li ₂ S-0.5SiS ₂	4.80E-5						312
0.985(0.5Li ₂ S-0.5SiS ₂)-0.015Li ₃ PO ₄	6.28E-5						312
0.975(0.5Li ₂ S-0.5SiS ₂)-0.025Li ₃ PO ₄	8.76E-5						312
0.95(0.5Li ₂ S-0.5SiS ₂)-0.05Li ₃ PO ₄	8.68E-5						312

0.9(0.5Li ₂ S-0.5SiS ₂)-0.1Li ₃ PO ₄	6.76E-5						312
0.6Li ₂ S-0.4SiS ₂	1.85E-4						312
0.99(0.6Li ₂ S-0.4SiS ₂)-0.01Li ₃ PO ₄	2.53E-4						312
0.97(0.6Li ₂ S-0.4SiS ₂)-0.03Li ₃ PO ₄	3.97E-4						312
0.95(0.6Li ₂ S-0.4SiS ₂)-0.05Li ₃ PO ₄	2.03E-4						312
0.9(0.6Li ₂ S-0.4SiS ₂)-0.1Li ₃ PO ₄	5.20E-5						312
0.61Li ₂ S-0.39SiS ₂	5.24E-4						312
0.99(0.61Li ₂ S-0.39SiS ₂)-0.01Li ₃ PO ₄	5.05E-4						312
0.985(0.61Li ₂ S-0.39SiS ₂)-0.015Li ₃ PO ₄	5.96E-4						312
0.98(0.61Li ₂ S-0.39SiS ₂)-0.02Li ₃ PO ₄	7.69E-4						312
0.975(0.61Li ₂ S-0.39SiS ₂)-0.025Li ₃ PO ₄	6.36E-4						312
0.97(0.61Li ₂ S-0.39SiS ₂)-0.03Li ₃ PO ₄	5.83E-4						312
0.95(0.61Li ₂ S-0.39SiS ₂)-0.05Li ₃ PO ₄	4.68E-4						312
0.9(0.61Li ₂ S-0.39SiS ₂)-0.1Li ₃ PO ₄	1.28E-4						312
0.99(0.65Li ₂ S-0.35SiS ₂)-0.01Li ₃ PO ₄	3.60E-4						312
0.97(0.65Li ₂ S-0.35SiS ₂)-0.03Li ₃ PO ₄	2.62E-4						312
0.95(0.65Li ₂ S-0.35SiS ₂)-0.05Li ₃ PO ₄	1.81E-4						312

0.9(0.65Li ₂ S-0.35SiS ₂)-0.1Li ₃ PO ₄	7.13E-5						312
0.7Li ₂ S-0.3P ₂ S ₅	5.2E-3						313
Lil	3.07E-7						314
0.998Lil-0.002Cal ₂	9.80E-7						314
0.99Lil-0.01Cal ₂	5.54E-6	0.43					314
Lil	2.74E-8	0.43					315
0.8Lil-0.2Al ₂ O ₃	6.84E-6	0.35					315
0.7Lil-0.3Al ₂ O ₃	2.07E-5	0.33					315
0.6Lil-0.4Al ₂ O ₃	3.94E-5	0.33					315
0.5Lil-0.5Al ₂ O ₃	2.58E-5	0.33					315
0.4Lil-0.6Al ₂ O ₃	6.76E-6	0.37					315
Li _{3.5} P _{0.5} Si _{0.5} O ₄	4.27E-7	0.57					19
Li _{3.5} P _{0.5} Ge _{0.5} O ₄	7.89E-6	0.56					19
Li _{3.5} As _{0.5} Si _{0.5} O ₄	4.05E-6	0.55					19
Li _{3.5} V _{0.5} Si _{0.5} O ₄	1.20E-5	0.53					19
Li _{3.5} As _{0.5} Ge _{0.5} O ₄	2.83E-5	0.51					19
Li _{3.5} V _{0.5} Ge _{0.5} O ₄	3.00E-5						19
Li _{3.5} As _{0.5} Ti _{0.5} O ₄	3.22E-5	0.52					19
Li _{3.5} As _{0.5} V _{0.5} O ₄	4.01E-5	0.49					19
LiHf ₂ (PO ₄) ₃ -0.1Li ₂ O	1.12E-4						19
LiHf ₂ (PO ₄) ₃ -0.2Li ₂ O	2.78E-5						19
LiHf ₂ (PO ₄) ₃ -0.3Li ₂ O	2.58E-5						19
LiHf ₂ (PO ₄) ₃ -0.4Li ₂ O	3.40E-5						19
LiTi ₂ (PO ₄) ₃	1.69E-6	0.30					316

0.95LiTi ₂ (PO ₄) ₃ - 0.05Li ₃ PO ₄	5.52E-5	0.29					316
0.9LiTi ₂ (PO ₄) ₃ - 0.1Li ₃ PO ₄	1.38E-4	0.28					316
0.8LiTi ₂ (PO ₄) ₃ - 0.2Li ₃ PO ₄	1.93E-4	0.31					316
0.7LiTi ₂ (PO ₄) ₃ - 0.3Li ₃ PO ₄	2.45E-4	0.30					316
0.95LiTi ₂ (PO ₄) ₃ - 0.05Li ₃ BO ₃	3.59E-5	0.30					316
0.9LiTi ₂ (PO ₄) ₃ - 0.1Li ₃ BO ₃	2.54E-4	0.30					316
0.8LiTi ₂ (PO ₄) ₃ - 0.2Li ₃ BO ₃	2.97E-4	0.30					316
0.7LiTi ₂ (PO ₄) ₃ - 0.3Li ₃ BO ₃	2.45E-4	0.29					316
0.5LiTi ₂ (PO ₄) ₃ - 0.5Li ₃ BO ₃	2.73E-5	0.31					316
LiTi ₂ (PO ₄) ₃	1.00E-4						317
LiTi ₂ (PO ₄) ₃ -0.15LiPO ₄	6.00E-4						317
LiTi ₂ (PO ₄) ₃ -0.3LiPO ₄	9.92E-4						317
LiTi ₂ (PO ₄) ₃ -0.6LiPO ₄	1.23E-3						317
LiTi ₂ (PO ₄) ₃ -0.9LiPO ₄	1.10E-3						317
LiTi ₂ (PO ₄) ₃ -0.15LiBO ₃	4.80E-4						317
LiTi ₂ (PO ₄) ₃ -0.3LiBO ₃	1.66E-3						317
LiTi ₂ (PO ₄) ₃ -0.6LiBO ₃	1.12E-3						317
LiTi ₂ (PO ₄) ₃ -0.9LiBO ₃	8.91E-4						317
LiTi ₂ (PO ₄) ₃ -1.5LiBO ₃	6.48E-4						317
LiTi ₂ (PO ₄) ₃ -0.2Li ₂ SO ₄	8.35E-4						317
LiTi ₂ (PO ₄) ₃ -0.4Li ₂ SO ₄	1.66E-3						317

$\text{LiTi}_2(\text{PO}_4)_3 \cdot 0.6\text{Li}_2\text{SO}_4$	5.67E-4						317
$\text{LiTi}_2(\text{PO}_4)_3 \cdot 0.4\text{LiCl}$	6.45E-4						317
$\text{LiTi}_2(\text{PO}_4)_3 \cdot 0.8\text{LiCl}$	1.28E-3						317
$\text{LiTi}_2(\text{PO}_4)_3 \cdot 1.2\text{LiCl}$	1.02E-3						317
$\text{LiTi}_2(\text{PO}_4)_3 \cdot 0.4\text{LiNO}_3$	1.18E-3						317
$\text{LiTi}_2(\text{PO}_4)_3 \cdot 0.8\text{LiNO}_3$	1.49E-3						317
$\text{LiTi}_2(\text{PO}_4)_3 \cdot 1.2\text{LiNO}_3$	9.95E-4						317
$\text{Li}_{0.39}\text{La}_{0.54}\text{TiO}_3$	1.08E-3	0.316					318
$(\text{Li}_{0.39}\text{La}_{0.54})_{1.006}\text{Al}_{0.006}\text{Ti}_{0.994}\text{O}_3$	1.13E-3	0.308					318
$(\text{Li}_{0.39}\text{La}_{0.54})_{1.01}\text{Al}_{0.02}\text{Ti}_{0.98}\text{O}_3$	1.58E-3	0.278					318
$(\text{Li}_{0.39}\text{La}_{0.54})_{1.03}\text{Al}_{0.06}\text{Ti}_{0.94}\text{O}_3$	1.39E-3	0.290					318
$(\text{Li}_{0.39}\text{La}_{0.54})_{1.005}\text{Cr}_{0.01}\text{Ti}_{0.99}\text{O}_3$	9.52E-4	0.300					318
$(\text{Li}_{0.39}\text{La}_{0.54})_{1.01}\text{Cr}_{0.02}\text{Ti}_{0.98}\text{O}_3$	1.01E-3	0.315					318
$(\text{Li}_{0.39}\text{La}_{0.54})_{1.025}\text{Cr}_{0.05}\text{Ti}_{0.95}\text{O}_3$	1.04E-3	0.298					318
$\text{La}_{0.51}\text{Li}_{0.34}\text{TiO}_{2.94}$	1E-3	0.38					319
$\text{La}_{0.57}\text{Li}_{0.26}\text{TiO}_{2.99}$	1E-3	0.34					319
$\text{La}_{0.6}\text{Li}_{0.16}\text{TiO}_{3.01}$	6.3E-4	0.33					319
$\text{La}_{0.64}\text{Li}_{0.067}\text{TiO}_3$	7.9E-5	0.36					319
$(\text{La}_{0.5}\text{Li}_{0.5})_{0.95}\text{Sr}_{0.05}\text{TiO}_3$	1.49E-3						319
$(\text{La}_{0.5}\text{Li}_{0.5})_{0.9}\text{Sr}_{0.1}\text{TiO}_3$	1.30E-3						319
$(\text{La}_{0.5}\text{Li}_{0.5})_{0.75}\text{Sr}_{0.25}\text{TiO}_3$	8.99E-5						319
$(\text{La}_{0.5}\text{Li}_{0.5})_{0.95}\text{Ba}_{0.05}\text{TiO}_3$	7.61E-4						319

$\text{La}_{0.63}\text{Li}_{0.1}\text{Mg}_{0.5}\text{W}_{0.5}\text{O}_3$	1.69E-6	0.39						319
$\text{Li}_{0.5}\text{La}_{0.5}\text{TiO}_3$	8.67E-4	0.28						320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.98}\text{Sn}_{0.02}\text{O}_3$	4.86E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.96}\text{Sn}_{0.04}\text{O}_3$	3.89E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.94}\text{Sn}_{0.06}\text{O}_3$	3.52E-4	0.294						320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.9}\text{Sn}_{0.1}\text{O}_3$	2.60E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.98}\text{Zr}_{0.02}\text{O}_3$	4.16E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.96}\text{Zr}_{0.04}\text{O}_3$	2.86E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.94}\text{Zr}_{0.06}\text{O}_3$	2.23E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.9}\text{Zr}_{0.1}\text{O}_3$	7.05E-5							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.998}\text{Mn}_{0.002}\text{O}_3$	9.12E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.996}\text{Mn}_{0.004}\text{O}_3$	9.64E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.994}\text{Mn}_{0.006}\text{O}_3$	1.08E-3							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.992}\text{Mn}_{0.008}\text{O}_3$	1.13E-3							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.99}\text{Mn}_{0.01}\text{O}_3$	1.13E-3							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.998}\text{Ge}_{0.002}\text{O}_3$	9.12E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.996}\text{Ge}_{0.004}\text{O}_3$	9.64E-4							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.994}\text{Ge}_{0.006}\text{O}_3$	1.08E-3							320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.992}\text{Ge}_{0.008}\text{O}_3$	1.13E-3	0.265						320
$\text{Li}_{0.5}\text{La}_{0.5}\text{Ti}_{0.99}\text{Ge}_{0.01}\text{O}_3$	1.13E-3							320
$\text{La}_{0.58}\text{Li}_{0.36}\text{Ti}_{0.95}\text{Mg}_{0.05}\text{O}_3$	2.1E-4	0.29						321
$\text{La}_{0.56}\text{Li}_{0.36}\text{Ti}_{0.95}\text{Al}_{0.05}\text{O}_3$	6.4E-4	0.26						321
$\text{La}_{0.55}\text{Li}_{0.36}\text{Ti}_{0.95}\text{Mn}_{0.05}\text{O}_3$	1.9E-4	0.29						321
$\text{La}_{0.55}\text{Li}_{0.36}\text{Ti}_{0.95}\text{Ge}_{0.05}\text{O}_3$	3.6E-4	0.29						321
$\text{La}_{0.55}\text{Li}_{0.36}\text{Ti}_{0.95}\text{Ru}_{0.05}\text{O}_3$	5.2E-5	0.28						321

$\text{La}_{0.51}\text{Li}_{0.36}\text{Ti}_{0.95}\text{W}_{0.05}\text{O}_3$	7.3E-4	0.27						321
$\text{La}_{0.55}\text{Li}_{0.36}\text{Ti}_{0.9}\text{W}_{0.1}\text{O}_3$	4.4E-4	0.27						321
$\text{La}_{0.55}\text{Li}_{0.36}\text{Ti}_{0.995}\text{Al}_{0.005}\text{O}_3$	1.1E-3	0.28						321
$\text{La}_{0.55}\text{Li}_{0.36}\text{Ti}_{0.992}\text{Al}_{0.008}\text{O}_3$	6.5E-4	0.29						321
$\text{La}_{0.54}\text{Li}_{0.36}\text{Ti}_{0.995}\text{W}_{0.005}\text{O}_3$	2.6E-4	0.30						321
$\text{La}_{0.54}\text{Li}_{0.36}\text{TiO}_3$	8.9E-4	0.29						321
$\text{La}_{0.606}\text{Li}_{0.06}\text{Ti}_{0.94}\text{Al}_{0.06}\text{O}_3$	1.68E-6	0.36						322
$\text{La}_{0.566}\text{Li}_{0.1}\text{Ti}_{0.9}\text{Al}_{0.1}\text{O}_3$	7.34E-6	0.35						322
$\text{La}_{0.516}\text{Li}_{0.15}\text{Ti}_{0.85}\text{Al}_{0.15}\text{O}_3$	9.66E-6	0.36						322
$\text{La}_{0.466}\text{Li}_{0.2}\text{Ti}_{0.8}\text{Al}_{0.2}\text{O}_3$	4.28E-5	0.33						322
$\text{La}_{0.416}\text{Li}_{0.25}\text{Ti}_{0.75}\text{Al}_{0.25}\text{O}_3$	7.66E-5	0.35						322
$\text{La}_{0.366}\text{Li}_{0.3}\text{Ti}_{0.7}\text{Al}_{0.3}\text{O}_3$	1.72E-5	0.33						322
$\text{Li}_{0.12}\text{La}_{0.63}\text{TiO}_3$	2.00E-4							323
$\text{Li}_{0.18}\text{La}_{0.61}\text{TiO}_3$	4.43E-4							323
$\text{Li}_{0.24}\text{La}_{0.59}\text{TiO}_3$	9.93E-4							323
$\text{Li}_{0.3}\text{La}_{0.57}\text{TiO}_3$	1.10E-3							323
$\text{Li}_{0.39}\text{La}_{0.54}\text{TiO}_3$	1.02E-3							323
$\text{Li}_{0.45}\text{La}_{0.52}\text{TiO}_3$	9.05E-4							323
$\text{LiZr}_2(\text{PO}_4)_3$	4.77E-7							324
$\text{Li}_{1.05}\text{Al}_{0.05}\text{Zr}_{1.9}(\text{PO}_4)_3$	5.79E-7							324
$\text{Li}_{1.1}\text{Al}_{0.1}\text{Zr}_{1.8}(\text{PO}_4)_3$	6.35E-7							324
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Zr}_{1.6}(\text{PO}_4)_3$	1.90E-6	0.48						324
$\text{Li}_{1.225}\text{Al}_{0.225}\text{Zr}_{1.55}(\text{PO}_4)_3$	2.13E-6	0.48						324
$\text{Li}_{1.25}\text{Al}_{0.25}\text{Zr}_{1.5}(\text{PO}_4)_3$	2.06E-6	0.48						324
$\text{Li}_{1.275}\text{Al}_{0.275}\text{Zr}_{1.45}(\text{PO}_4)_3$	3.05E-6	0.48						324

$\text{Li}_{1.3}\text{Al}_{0.3}\text{Zr}_{1.4}(\text{PO}_4)_3$	1.91E-6	0.48						324
$\text{LiHf}_2(\text{PO}_4)_3$	3.42E-6							325
$\text{LiHfTi}(\text{PO}_4)_3$	5.63E-7							325
$\text{Li}_{0.1}\text{Zr}_{1.1}\text{Nb}_{0.9}\text{P}_3\text{O}_{12}$	6E-6							325
$\text{LiTi}_2(\text{PO}_4)_3$	1.04E-7							326
$\text{Li}_{1.1}\text{Sc}_{0.1}\text{Ti}_{1.9}(\text{PO}_4)_3$	1.75E-5							326
$\text{Li}_{1.2}\text{Sc}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	4.11E-5	0.34						326
$\text{Li}_{1.3}\text{Sc}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	4.06E-5							326
$\text{Li}_{1.4}\text{Sc}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	9.43E-6							326
$\text{Li}_{1.5}\text{Sc}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$	5.42E-7							326
$\text{Li}_{1.1}\text{Y}_{0.1}\text{Ti}_{1.9}(\text{PO}_4)_3$	2.94E-7							326
$\text{Li}_{1.2}\text{Y}_{0.2}\text{Ti}_{1.8}(\text{PO}_4)_3$	7.95E-7							326
$\text{Li}_{1.3}\text{Y}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	1.01E-6	0.40						326
$\text{Li}_{1.4}\text{Y}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	2.97E-7							326
$\text{LiTi}_2(\text{PO}_4)_3\text{-}0.5\text{LiF}$	2.318E-4	0.28						327
$\text{LiTi}_2(\text{PO}_4)_3$	7.181E-6	0.48						327
$14\text{Li}_2\text{O}\text{-}9\text{Al}_2\text{O}_3\text{-}38\text{TiO}_2\text{-}39\text{P}_2\text{O}_5$	1.3E-3	0.33						328
$\text{Li}_{6.6}\text{La}_3\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	3.13E-4	0.38						329
$\text{Li}_{6.6}\text{La}_{2.875}\text{Y}_{0.125}\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	3.17E-4	0.35						329
$\text{Li}_{6.6}\text{La}_{2.75}\text{Y}_{0.25}\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	4.36E-4	0.34						329
$\text{Li}_{6.6}\text{La}_{2.5}\text{Y}_{0.5}\text{Zr}_{1.6}\text{Ta}_{0.4}\text{O}_{12}$	2.26E-4	0.39						329
Li_2ZrS_3	7.3E-6							330
$\text{Li}_{2.2}\text{Zn}_{0.1}\text{Zr}_{0.9}\text{S}_3$	1.2E-4							330

0.7Li ₂ S-0.3P ₂ S ₅	8.1E-5	0.425						12
Li ₇ PS ₆	1.61E-6	0.16						176

II. Labels for comparing all descriptors-simplification combinations

A subset of the digitized labels was used for comparing between the different semi-supervised learning models. In total, the label subset is comprised of 155 structures. The subset is required because not all structures are compatible with all the descriptor transformations. Some descriptor-structure combinations produce coding errors, imaginary values, or infinite values. To directly compare all the descriptors, it's necessary to have a common set of labels. The 155 labels that worked for all descriptors is listed in the subsequent table:

Compound	$\sigma_{25^\circ\text{C}}$ (S cm ⁻¹)	E_a (eV)	Space Group	Space Group #	Other names	ICSD	Citation
Li ₄ P ₂ O ₇	<1E-10	1.617	P $\bar{1}$	2		248414	8
Li ₇ P ₃ S ₁₁	3.2E-3	0.124	P $\bar{1}$	2		157654	5
Li ₇ BiO ₆	8.80E-07	0.58	P $\bar{1}$	2		155950	3
Li ₇ SbO ₆	6.70E-08	0.7	P $\bar{1}$	2		413370	3
Li ₆ CuB ₄ O ₁₀	1.00E-13	0.92	P $\bar{1}$	2	β -Li ₆ CuB ₄ O ₁₀	4819	10
LiAlSi ₃ O ₈	1.30E-10		C $\bar{1}$	2		81980	1
Li ₃ BP ₂ O ₈	9.60E-12	0.62	P $\bar{1}$	2		248343	7
LiSn ₂ (PO ₄) ₃	2.04E-9		P $\bar{1}$	2		83832	2
LiV(PO ₄)F	8.1E-7	0.23	P $\bar{1}$	2		183876	6
Li ₂ NaBP ₂ O ₈	4.40E-18	1.21	P $\bar{1}$	2		291512	7
LiMgSO ₄ F	5.40E-08	0.54	P $\bar{1}$	2		281119	9
Li ₂ ZnGeO ₄	1.00E-07	0.4	Pc	7		34362	13
Li ₄ SiO ₄	5.00E-10	0.55	P2 ₁ /m	11		238603	17
Li _{3.7} P _{0.3} Si _{0.7} O ₄	3.84E-7		P2 ₁ /m	11		35168	19
Li _{7.22} Si _{1.5} P _{0.5} O ₈	1.64E-7	0.48	P2 ₁ /m	11		238602	16
Li ₃ InCl ₆	2.04E-3	0.35	C2/m	12		89617	20
Li ₂ P ₂ S ₆	7.80E-11	0.48	C2/m	12		253894	21
LiPO ₃	1.00E-09		P2/c	13		51630	28

LiAlSi ₄ O ₁₀	1.01E-10		P2/c	13		194284	1
LaLiO ₂	<1E-10	0.92	P2 ₁ /c	14		239278	36
LiBO ₂	1.00E-08	0.71	P2 ₁ /c	14		200891	34
LiSbO ₂	<1E-10	0.88	P2 ₁ /c	14		262075	39
LiYO ₂	1.80E-08	0.72	P2 ₁ /c	14		45511	33
LiAlCl ₄	1.00E-06	0.47	P2 ₁ /c	14		35275	32
Li ₃ BO ₃	7.40E-11	0.63	P2 ₁ /c	14		9105	30
Li ₂ SO ₄	1.40E-14	1.1	P2 ₁ /c	14		2512	29
Li ₆ Ge ₂ O ₇	8.50E-07	0.43	P2 ₁ /c	14		31050	31
LiGaBr ₄	7.00E-6	0.54	P2 ₁ /c	14		61337	25
Li ₄ Zn(PO ₄) ₂	<1E-10	1.3	P2 ₁ /c	14	α -Li ₄ Zn(P O ₄) ₂	255464	38
La(Li _{0.76} Mg _{0.08})O ₂	7.27E-10	0.66	P2 ₁ /c	14		239280	36
(La _{0.9} Sr _{0.1})LiO ₂	6.29E-10	0.62	P2 ₁ /c	14		239279	36
Li ₂ Sr ₂ Al(PO ₄) ₃	<1E-10	1.02	P2 ₁ /c	14		431319	40
Li _{2.5} V ₂ (PO ₄) ₃	1.9E-7		P2 ₁ /c	14		240269	37
Li ₂ SnS ₃	1.50E-05	0.59	C2/c	15		251656	43
LiVO ₃	2.048E-9		C2/c	15		51443	48
Li ₆ Zr ₂ O ₇	5.20E-10	0.68	C2/c	15		73835	41
Li ₃ AlF ₆	5.00E-07	0.54	C2/c	15		85171	42
LiTa ₂ PO ₈	1.6E-3	0.32	C2/c	15		267438	44
LiBaP ₂ O ₇	1.00E-10		C2/c	15		280927	45
Li ₃ Na ₅ (TiS ₄) ₂	8.80E-06	0.4	C2/c	15		391258	46
LiGd(PO ₃) ₄	<1E-10	1.7	C2/c	15		416442	47
Li _{3.7} Zn _{0.7} Ga _{0.3} (PO ₄) ₂	<1E-10	0.91	P2 ₁ 2 ₁ 2 ₁	19	β' -Li _{3.7} Zn _{0.7}	255466	38

					$\text{Ga}_{0.3}(\text{P}_\text{O}_4)_2$		
Li_3SbS_4	1.5E-6	0.518	$\text{Pmn}2_1$	31		8407	51
Li_3PS_4	2.60E-07	0.49	$\text{Pmn}2_1$	31	$\gamma\text{-Li}_3\text{PS}_4$	180318	52
Li_3SbS_3	1.00E-07	0.4	$\text{Pna}2_1$	33		424834	55
LiGaO_2	2.40E-14	0.86	$\text{Pna}2_1$	33		18152	53
$\text{LiB}_6\text{O}_9\text{F}$	5.40E-24	1.38	$\text{Pna}2_1$	33		420286	54
LiSi_2N_3	6.17E-08	0.64	$\text{Cmc}2_1$	36		34118	56
$\text{Li}_2(\text{PO}_2\text{N})$	<1E-10	0.57	$\text{Cmc}2_1$	36		188493	57
$\text{LiGa}_2\text{GeS}_6$	3.80E-08	0.47	$\text{Fdd}2$	43		254406	58
Li_5AlO_4	5.00E-10	0.99	Pmmn	59		16229	64
$\text{Li}_{14}\text{Nd}_5(\text{Si}_{11}\text{N}_{19}\text{O}_5)\text{O}_2\text{F}_2$	1.7E-10	0.69	Pmmn	59		262923	65
Li_2SiN_2	1.60E-07		Pbca	61		420126	66
Li_5GaO_4	5.00E-09	0.71	Pbca	61	$\alpha\text{-Li}_5\text{GaO}_4$	9082	64
Li_3PS_4	1.60E-04	0.36	Pnma	62	$\beta\text{-Li}_3\text{PS}_4$	180319	52
Li_3PO_4	4.2E-18	1.24	Pnma	62	$\gamma\text{-Li}_3\text{PO}_4$	79427	70
Li_3PO_4	<1E-10	1.14	Pnma	62	$\gamma\text{-Li}_3\text{PO}_4$	20208	68
Li_4SnS_4	7.0E-5	0.29	Pnma	62		290832	80
Li_4SnSe_4	2E-5	0.45	Pnma	62		193768	76
Li_4GeS_4	2.00E-07	0.53	Pnma	62		290831	79
Li_4GeS_4	2E-7	0.53	Pnma	62		92200	71
Li_2ZnI_4	4.00E-08	0.58	Pnma	62		402062	81
$\text{Li}_{3.5}\text{Ge}_{0.5}\text{V}_{0.5}\text{O}_4$	1.77E-5		Pnma	62		66576	84
$\text{Li}_{6.6}\text{SiPO}_8$	1.48E-7	0.49	Pnma	62		238601	16
$\text{Li}_{3.75}\text{Ge}_{0.75}\text{V}_{0.25}\text{O}_4$	5.66E-6		Pnma	62		150918	73

$\text{Li}_4\text{Zn}(\text{PO}_4)_2$	<1E-10	1.1	Pnma	62	$\beta\text{-Li}_4\text{Zn}(\text{PO}_4)_2$	255465	38
$\text{Li}_{2.88}\text{PO}_{3.73}\text{N}_{0.14}$	1.4E-13	0.97	Pnma	62		79426	70
$\text{Li}_2\text{Mg}_2(\text{MoO}_4)_3$	<1E-10	0.71	Pnma	62		170956	75
$\text{Li}_{3.70}\text{Ge}_{0.85}\text{W}_{0.15}\text{O}_4$	3.80E-5		Pnma	62		150920	73
$\text{Li}_{14}\text{Zn}(\text{GeO}_4)_4$	1.00E-06	0.24	Pnma	62		100169	72
$\text{Nd}_{0.54}\text{Li}_{0.36}\text{TiO}_3$	3.42E-8	0.50	Pnma	62		81047	86
$\text{Li}_{6.5}\text{O}_8\text{P}_{1.5}\text{Si}_{0.5}$	4.49E-07	0.44	Pnma	62		238600	16
$\text{Pr}_{0.51}\text{Li}_{0.39}\text{TiO}_{2.96}$	5.34E-7	0.44	Pnma	62		81048	86
LiZnSO_4F	2.80E-05	0.2455	Pnma	62		261343	78
$\text{Li}_{3.5}\text{Zn}_{0.5}\text{Ga}_{0.5}(\text{PO}_4)_2$	<1E-10	1.02	Pnma	62	$\beta\text{-Li}_{3.5}\text{Zn}_{0.5}\text{Ga}_{0.5}(\text{PO}_4)_2$	255468	38
$\text{Li}_4\text{H}_8\text{Cl}_4\text{O}_4$	1E-8	0.777	Cmcm	63	$\text{LiCl}^*\text{H}_2\text{O}$	281198	88
Li_2MgBr_4	7.80E-10	0.77	Cmmm	65		73276	89
$\text{Li}_{0.18}\text{La}_{0.61}\text{TiO}_3$	2.0E-4	0.432	Cmmm	65		99398	90
LiBiO_2	3.80E-08	0.1	Ibam	72		46022	30
LiZnPS_4	5.4E-8		I $\bar{4}$	82		95785	69
$(\text{Li}_{1.19}\text{Zn}_{0.9})\text{PS}_4$	0.65E-5	0.25	I $\bar{4}$	82		264463	69
$(\text{Li}_{1.69}\text{Zn}_{0.66})\text{PS}_4$	1.30E-4	0.181	I $\bar{4}$	82		264462	69
$(\text{Li}_{0.5}\text{Ce}_{0.5})(\text{MoO}_4)$	1.3E-8	0.4	I4 ₁ /a	88		186450	91
$(\text{Li}_{0.5}\text{Ce}_{0.25}\text{Sm}_{0.25})(\text{MoO}_4)$	1.8E-10	0.5	I4 ₁ /a	88		186452	91
$(\text{Li}_{0.5}\text{Ce}_{0.25}\text{Pr}_{0.25})(\text{MoO}_4)$	1E-9	0.5	I4 ₁ /a	88		186451	91
Li_2TeO_4	<1E-10	1.129	P4 ₁ 22	91		1485	92
Li_3BN_2	1.60E-10	0.67	P4 ₂ 2 ₁ 2	94	$\alpha\text{-Li}_3\text{BN}_2$	655673	93

$\text{Li}_2\text{B}_4\text{O}_7$	1.00E-10		I4 ₁ cd	110		65930	94
$\text{La}_{0.52}\text{Li}_{0.45}\text{TiO}_3$	5.01E-4		P4/mmm	123		50434	97
$\text{Li}(\text{NdTiO}_4)$	<1E-10	0.87	P4/nmmZ	129		91844	99
$\text{Li}_4\text{PS}_4\text{I}$	1.2E-4	0.37	P4/nmmZ	129		432169	101
$\text{Li}(\text{LaTiO}_4)$	<1E-10	0.83	P4/nmmZ	129		91843	99
$\text{La}_{0.62}\text{Li}_{0.14}(\text{Mg}_{0.5}\text{W}_{0.5})\text{O}_3$	1.2E-5	0.37	P4/nmm	129		151902	100
Li_6ZnO_4	9.40E-09	0.61	P4 ₂ /nmc	137		62137	64
$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	7E-3	0.27	P4 ₂ /nmc C	137		193755	107
$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	3.98E-3	0.305	P4 ₂ /nmc	137		255750	108
$\text{Li}_{10}\text{GePS}_{12}$	1.21E-2		P4 ₂ /nmc	137		188887	104
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	2.46E-2	0.274	P4 ₂ /nmc	137		241439	108
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	1.20E-02	0.25	P4 ₂ /nmc	137		255749	110
$\text{Li}_{10.35}\text{Ge}_{1.35}\text{P}_{1.65}\text{S}_{12}$	1.44E-2	0.269	P4 ₂ /nmc S	137		193947	104
$\text{Li}_{10.35}\text{Si}_{1.35}\text{P}_{1.65}\text{S}_{12}$	6.5E-3		P4 ₂ /nmcS	137		252037	109
$\text{Li}_{9.81}\text{Sn}_{0.81}\text{P}_{2.19}\text{S}_{12}$	5.5E-3		P4 ₂ /nmc	137		252040	109
$\text{Li}_{10.2}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.2}\text{P}_{1.8}\text{S}_{12}$	7.82E-3		P4 ₂ /nmcS	137		5667	111
$\text{Li}_{10.2}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.2}\text{P}_{1.8}\text{S}_{12}$	2.69E-3		P4 ₂ /nmcS	137		257948	111
$\text{Li}_{10.5}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.5}\text{P}_{1.5}\text{S}_{12}$	8.79E-3		P4 ₂ /nmcS	137		5668	111
$\text{Li}_{10}(\text{Ge}_{0.776}\text{Sn}_{0.224})\text{P}_2\text{S}_{12}$	1.41E-2	0.276	P4 ₂ /nmc	137		255748	108
$\text{LiLaNb}_2\text{O}_7$	<1E-8		I4/mmm	139		72566	114
$\text{Li}_4\text{Sr}_3\text{Nb}_6\text{O}_{20}$	<1E-10		I4/mmm	139		87824	115
$\text{Li}_4\text{Sr}_{3.056}\text{Nb}_6\text{O}_{20}$	<1E-10	0.74	I4/mmm	139		109168	115
$\text{Li}_4\text{Sr}_3\text{Nb}_{5.77}\text{Fe}_{0.23}\text{O}_{19.77}$	<1E-10		I4/mmm	139		87823	115
Li_4SrN_2	2.30E-13	0.9	I4 ₁ /amd	141		87413	116

<chem>LiAlO2</chem>	1.10E-12	0.97	I4 ₁ /amd	141	r-LiAlO ₂	99517	33
<chem>LiScO2</chem>	<1E-10	1.047	I4 ₁ /amd	141		257819	117
<chem>LiScO2</chem>	1.00E-12	0.87	I4 ₁ /amd	141		36124	33
<chem>Li0.9Sc0.9Zr0.1O2</chem>	<1E-10	0.912	I4 ₁ /amd	141		257820	117
<chem>Li7La3Zr2O12</chem>	1.63E-6	0.54	I4 ₁ /acdZ	142	"tetraganol-LLZO"	183684	119
<chem>LiAlGeO4</chem>	<1E-10	0.97	R3H	146		257741	123
<chem>LiGaSiO4</chem>	3.00E-16	0.9	R3H	146		65125	122
<chem>LiGa0.5Al0.5GeO4</chem>	<1E-10	1.06	R3H	146		257740	123
<chem>LiNaSO4</chem>	8.80E-10		P31c	159		14364	125
<chem>Li5NCl2</chem>	1.20E-06	0.5	R̄3m	166		84763	131
<chem>LiGe2(PO4)3</chem>	4.83E-9	0.654	R̄3cH	167		69763	133
<chem>LiZr2(PO4)3</chem>	2.96E-10		R̄3cH	167		201935	2
<chem>LiTi2(PO4)3</chem>	7.61E-6	0.38	R̄3cH	167		95979	132
<chem>LiGe2(PO4)3</chem>	3.33E-7		R̄3cH	167		263767	2
<chem>Li1.3(Al0.23Y0.07Ti1.7)(PO4)3</chem>	3.84E-8		R̄3cH	167		253243	138
<chem>Li9Mg3(PO4)4F3</chem>	<1E-10	0.835	P6 ₃	173		426103	148
<chem>LiLa9Si6O26</chem>	<1E-10		P6 ₃ /m	176		291218	150
<chem>Li0.284Sm4.512Si3O12.91</chem>	<1E-10		P6 ₃ /m	176		83279	150
<chem>Pb6.12Ca1.9Li1.96(PO4)6</chem>	<1E-10	1.05	P6 ₃ /m	176		59615	149
<chem>Li5La3Nb2O12</chem>	8E-6	0.43	I2 ₁ 3	199		54865	159
<chem>(K0.1Li0.9)(SbO3)</chem>	1.36E-8		Pn̄3Z	201		200984	160
<chem>Li2CoTi3O8</chem>	<1E-10	1.33	P4 ₃ 2	212		86166	163
<chem>Li2ZnGe3O8</chem>	<1E-10	2.14	P4 ₃ 2	212		86169	163
<chem>Li2MgTi3O8</chem>	<1E-10	0.71	P4 ₃ 2	212		86165	163

(Li _{0.55} Mg _{0.45})(Li _{0.445} Mg _{0.0} ₅₅)Ti _{1.5} O ₄	1.53E-11	0.786	P4 ₃ 2	212		168145	164
(Li _{0.61} Mg _{0.39})(Li _{0.46} Mg _{0.00} ₅ Ti _{0.035})Ti _{1.5} O ₄	6.56E-10	0.685	P4 ₃ 2	212		168144	164
Li ₂ VCl ₄	6.95E-6		F43m	216		74959	166
Li ₅ NiI ₂	4.00E-6		F43m	216		16800	165
Li ₆ PO ₅ Cl	5.54E-10	0.66	F43m	216		421479	173
Li ₇ PN ₄	1.60E-07	0.4	P43n	218		69017	95
Li ₉ NS ₃	8.30E-07	0.52	Pm $\bar{3}$ m	221		240749	185
Li ₃ OBr	1.10E-06	0.74	Pm $\bar{3}$ m	221		67265	194,195
Li ₂ (OH)Br	1.20E-6	0.75	Pm $\bar{3}$ m	221		200874	184
LiI	1E-7		Fm $\bar{3}$ m	225		414244	197
Li _{7.2} N _{1.6} Cl _{2.4}	8.4E-7	0.49	Fm $\bar{3}$ m	225		49646	131
Li _{0.19} La _{0.67} (Ti _{0.9} Co _{0.1})O ₃	1.08E-4		Fm $\bar{3}$ m	225		151535	182
LiCdCl ₄	5.80E-07	0.44	Fd $\bar{3}$ m	227		74958	199
Li ₂ MnCl ₄	4.79E-6		Fd $\bar{3}$ m	227		69678	166
Li ₂ MgCl ₄	6.24E-7		Fd $\bar{3}$ m	227		74957	166
LiSrTa ₂ O ₆ F	<1E-10	0.604	Fd $\bar{3}$ m	227		236010	200
Li _{1.9} Mn _{0.9} Ga _{0.1} Cl ₄	2.37E-7		Fd $\bar{3}$ m	227		50305	198
Li(Li _{0.34} Ti _{1.66})O ₄	6.03E-8	0.506	Fd $\bar{3}$ m	227		168137	164
(Li _{0.74} Mg _{0.26})(Li _{0.40} Mg _{0.04} Ti _{1.56})O ₄	1.51E-9	0.639	Fd $\bar{3}$ m	227		168142	164
(Li _{0.826} Mg _{0.174})(Li _{0.374} Mg _{0.026} Ti _{1.60})O ₄	4.24E-9	0.615	Fd $\bar{3}$ m	227		168141	164

III. Labels used for the final SOAP model

Once the best-performing descriptor-simplification is identified, an expanded set of labels can be employed. The mathematical transformation for the SOAP descriptor is compatible with most of the ~26,000 structures. In addition to the 155 labels used for descriptor comparisons, 64 labels were added. The full list of labels is included in the table below:

Compound	$\sigma_{25^\circ\text{C}}$ (S cm ⁻¹)	E_a (eV)	Space Group	Space Group #	Other names	ICSD	Citation
Li ₄ P ₂ O ₇	<1E-10	1.617	P $\bar{1}$	2		248414	8
Li ₇ P ₃ S ₁₁	3.2E-3	0.124	P $\bar{1}$	2		157654	5
Li ₇ BiO ₆	8.80E-07	0.58	P $\bar{1}$	2		155950	3
Li ₇ SbO ₆	6.70E-08	0.7	P $\bar{1}$	2		413370	3
Li ₆ CuB ₄ O ₁₀	1.00E-13	0.92	P $\bar{1}$	2	β - Li ₆ CuB ₄ O ₁₀	4819	10
LiAlSi ₃ O ₈	1.30E-10		C $\bar{1}$	2		81980	1
Li ₃ BP ₂ O ₈	9.60E-12	0.62	P $\bar{1}$	2		248343	7
LiSn ₂ (PO ₄) ₃	2.04E-9		P $\bar{1}$	2		83832	2
LiV(PO ₄)F	8.1E-7	0.23	P $\bar{1}$	2		183876	6
LiMgSO ₄ F	5.40E-08	0.54	P $\bar{1}$	2		281119	9
Li ₂ NaBP ₂ O ₈	4.40E-18	1.21	P $\bar{1}$	2		291512	7
Li ₂ ZnGeO ₄	1.00E-07	0.4	Pc	7		34362	13
Li ₄ SiO ₄	5.00E-10	0.55	P2 ₁ /m	11		238603	17
Li ₄ SiS ₄	5.00E-08	0.56	P2 ₁ /m	11		59708	15
Li _{3.7} P _{0.3} Si _{0.7} O ₄	3.84E-7		P2 ₁ /m	11		35168	19
Li _{7.22} Si _{1.5} P _{0.5} O ₈	1.64E-7	0.48	P2 ₁ /m	11		238602	16
Li ₂ P ₂ S ₆	7.80E-11	0.48	C2/m	12		253894	21
Li ₃ InCl ₆	2.04E-3	0.35	C2/m	12		89617	20
Li ₁₇ Sb ₁₃ S ₂₈	1.05E-9	0.4	C2/m	12		429902	24

LiPO ₃	1.00E-09		P2/c	13		51630	28
LiAlSi ₄ O ₁₀	1.01E-10		P2/c	13		194284	1
LaLiO ₂	<1E-10	0.92	P2 ₁ /c	14		239278	36
LiBO ₂	1.00E-08	0.71	P2 ₁ /c	14		200891	34
LiSbO ₂	<1E-10	0.88	P2 ₁ /c	14		262075	39
LiYO ₂	1.80E-08	0.72	P2 ₁ /c	14		45511	33
Li ₃ BO ₃	7.40E-11	0.63	P2 ₁ /c	14		9105	30
Li ₂ SO ₄	1.40E-14	1.1	P2 ₁ /c	14		2512	29
LiGaBr ₄	7.00E-6	0.54	P2 ₁ /c	14		61337	25
LiAlCl ₄	1.00E-06	0.47	P2 ₁ /c	14		35275	32
Li ₆ Ge ₂ O ₇	8.50E-07	0.43	P2 ₁ /c	14		31050	31
Li ₄ Zn(PO ₄) ₂	<1E-10	1.3	P2 ₁ /c	14	α - Li ₄ Zn(P O ₄) ₂	255464	38
Li _{2.5} V ₂ (PO ₄) ₃	1.9E-7		P2 ₁ /c	14		240269	37
La(Li _{0.76} Mg _{0.08})O ₂	7.27E-10	0.66	P2 ₁ /c	14		239280	36
(La _{0.9} Sr _{0.1})LiO ₂	6.29E-10	0.62	P2 ₁ /c	14		239279	36
Li ₂ Sr ₂ Al(PO ₄) ₃	<1E-10	1.02	P2 ₁ /c	14		431319	40
LiClC ₃ H ₇ NO	1.6E-4	0.881	P2 ₁ /c	14		238683	35
Li ₂ CrCl ₄	<1E-10	1.22	C2/c	15		202627	49
Li ₂ ZrO ₃	6.10E-10	0.78	C2/c	15		94894	33
Li ₆ Zr ₂ O ₇	5.20E-10	0.68	C2/c	15		73835	41
Li ₃ AlF ₆	5.00E-07	0.54	C2/c	15		85171	42
Li ₂ SnS ₃	1.50E-05	0.59	C2/c	15		251656	43
LiVO ₃	2.048E-9		C2/c	15		51443	48
LiTa ₂ PO ₈	1.6E-3	0.32	C2/c	15		267438	44

LiBaP ₂ O ₇	1.00E-10		C2/c	15		280927	45
LiGd(PO ₃) ₄	<1E-10	1.7	C2/c	15		416442	47
Li ₃ Na ₅ (TiS ₄) ₂	8.80E-06	0.4	C2/c	15		391258	46
Li _{3.7} Zn _{0.7} Ga _{0.3} (PO ₄) ₂	<1E-10	0.91	P2 ₁ 2 ₁ 2 ₁	19	β'- Li _{3.7} Zn _{0.7} Ga _{0.3} (P O ₄) ₂	255466	38
Li ₃ SbS ₄	1.5E-6	0.518	Pmn2 ₁	31		8407	51
Li ₃ PS ₄	2.60E-07	0.49	Pmn2 ₁	31	γ-Li ₃ PS ₄	180318	52
Li ₃ SbS ₃	1.00E-07	0.4	Pna2 ₁	33		424834	55
LiGaO ₂	2.40E-14	0.86	Pna2 ₁	33		18152	53
LiB ₆ O ₉ F	5.40E-24	1.38	Pna2 ₁	33		420286	54
LiSi ₂ N ₃	6.17E-08	0.64	Cmc2 ₁	36		34118	56
Li ₂ (PO ₂ N)	<1E-10	0.57	Cmc2 ₁	36		188493	57
LiGa ₂ GeS ₆	3.80E-08	0.47	Fdd2	43		254406	58
La _{0.595} Li _{0.215} TiO ₃	8.53E-4		Pmmm	47		92234	59
La _{0.62} Li _{0.14} TiO ₃	4.42E-4		Pmmm	47		92231	59
La _{0.64} Li _{0.08} TiO ₃	3.35E-4		Pmmm	47		92228	59
Li _{0.02} Na _{0.48} La _{0.5} Nb ₂ O ₆	3.99E-6		Pmmm	47		180635	60
Li _{0.04} Na _{0.46} La _{0.5} Nb ₂ O ₆	5.91E-6		Pmmm	47		180634	60
Li _{0.07} Na _{0.43} La _{0.5} Nb ₂ O ₆	1.23E-5		Pmmm	47		180633	60
Li _{0.1} Na _{0.4} La _{0.5} Nb ₂ O ₆	1.21E-5		Pmmm	47		180632	60
Li _{0.2} Na _{0.3} La _{0.5} Nb ₂ O ₆	1.18E-5		Pmmm	47		180631	60
Li _{0.3} Na _{0.2} La _{0.5} Nb ₂ O ₆	1.11E-5		Pmmm	47		180630	60
Li _{0.4} Na _{0.1} La _{0.5} Nb ₂ O ₆	9.92E-6		Pmmm	47		180629	60
Li ₅ AlO ₄	5.00E-10	0.99	Pmmn	59		16229	64
Li ₁₄ Nd ₅ (Si ₁₁ N ₁₉ O ₅)O ₂ F ₂	1.7E-10	0.69	Pmmn	59		262923	65

Li ₂ SiN ₂	1.60E-07		Pbca	61		420126	66
Li ₅ GaO ₄	5.00E-09	0.71	Pbca	61	α -Li ₅ GaO ₄	9082	64
Li ₃ PO ₄	4.2E-18	1.24	Pnma	62	γ -Li ₃ PO ₄	79427	70
Li ₃ PO ₄	<1E-10	1.14	Pnma	62	γ -Li ₃ PO ₄	20208	68
Li ₃ PS ₄	1.60E-04	0.36	Pnma	62	β -Li ₃ PS ₄	180319	52
Li ₄ SnS ₄	7.0E-5	0.29	Pnma	62		290832	80
Li ₄ SnSe ₄	2E-5	0.45	Pnma	62		193768	76
Li ₄ GeS ₄	2.00E-07	0.53	Pnma	62		290831	79
Li ₄ GeS ₄	2E-7	0.53	Pnma	62		92200	71
Li(BH ₄)	1E-8		Pnma	62		239763	77
Li ₂ ZnI ₄	4.00E-08	0.58	Pnma	62		402062	81
Li ₄ Zn(PO ₄) ₂	<1E-10	1.1	Pnma	62	β -Li ₄ Zn(P O ₄) ₂	255465	38
Li ₂ Mg ₂ (MoO ₄) ₃	<1E-10	0.71	Pnma	62		170956	75
Li _{0.2} Ca _{0.4} TaO ₃	3.53E-9	0.54	Pnma	62		151936	74
Li _{3.5} Ge _{0.5} V _{0.5} O ₄	1.77E-5		Pnma	62		66576	84
Li _{3.75} Ge _{0.75} V _{0.25} O ₄	5.66E-6		Pnma	62		150918	73
Li ₁₄ Zn(GeO ₄) ₄	1.00E-06	0.24	Pnma	62		100169	72
Li _{3.70} Ge _{0.85} W _{0.15} O ₄	3.80E-5		Pnma	62		150920	73
Li _{6.6} SiPO ₈	1.48E-7	0.49	Pnma	62		238601	16
Li _{2.88} PO _{3.73} N _{0.14}	1.4E-13	0.97	Pnma	62		79426	70
Li _{6.5} O ₈ P _{1.5} Si _{0.5}	4.49E-07	0.44	Pnma	62		238600	16
Nd _{0.54} Li _{0.36} TiO ₃	3.42E-8	0.50	Pnma	62		81047	86
Pr _{0.51} Li _{0.39} TiO _{2.96}	5.34E-7	0.44	Pnma	62		81048	86

LiZnSO ₄ F	2.80E-05	0.2455	Pnma	62		261343	78
Li _{3.5} Zn _{0.5} Ga _{0.5} (PO ₄) ₂	<1E-10	1.02	Pnma	62	β-Li _{3.5} Zn _{0.5} Ga _{0.5} (PO ₄) ₂	255468	38
Li _{0.2} (Ca _{0.36} Sr _{0.04})TaO ₃	9.2E-9		Pnma	62		151937	74
Li ₄ GeO ₄	2.80E-10	0.73	Cmcm	63		18096	87
Li ₄ H ₈ Cl ₄ O ₄	1E-8	0.777	Cmcm	63	LiCl*H ₂ O	281198	88
Li ₂ MgBr ₄	7.80E-10	0.77	Cmmm	65		73276	89
Li _{0.18} La _{0.61} TiO ₃	2.0E-4	0.432	Cmmm	65		99398	90
LiBiO ₂	3.80E-08	0.1	Ibam	72		46022	30
LiZnPS ₄	5.4E-8		I <bar{4}< td=""><td>82</td><td></td><td>95785</td><td>69</td></bar{4}<>	82		95785	69
(Li _{1.19} Zn _{0.9})PS ₄	0.65E-5	0.25	I <bar{4}< td=""><td>82</td><td></td><td>264463</td><td>69</td></bar{4}<>	82		264463	69
(Li _{1.69} Zn _{0.66})PS ₄	1.30E-4	0.181	I <bar{4}< td=""><td>82</td><td></td><td>264462</td><td>69</td></bar{4}<>	82		264462	69
(Li _{0.5} Ce _{0.5})(MoO ₄)	1.3E-8	0.4	I4 ₁ /a	88		186450	91
(Li _{0.5} Ce _{0.25} Sm _{0.25})(MoO ₄)	1.8E-10	0.5	I4 ₁ /a	88		186452	91
(Li _{0.5} Ce _{0.25} Pr _{0.25})(MoO ₄)	1E-9	0.5	I4 ₁ /a	88		186451	91
Li ₂ TeO ₄	<1E-10	1.129	P4 ₁ 22	91		1485	92
Li ₃ BN ₂	1.60E-10	0.67	P4 ₂ 2 ₁ 2	94	α-Li ₃ BN ₂	655673	93
Li ₂ B ₄ O ₇	1.00E-10		I4 ₁ cd	110		65930	94
LiY(BH ₄) ₄	1.26E-6		P <bar{4}2c< td=""><td>112</td><td></td><td>239762</td><td>77</td></bar{4}2c<>	112		239762	77
LiPN ₂	1.6E-7	0.40	I <bar{4}2d< td=""><td>122</td><td></td><td>66007</td><td>95</td></bar{4}2d<>	122		66007	95
Li _{0.33} La _{0.5} TiO ₃	1E-3	0.15	P4/mmm	123		82671	96
La _{0.5} Li _{0.5} TiO ₃	9.25E-4	0.39	P4/mmm	123		92236	59
La _{0.52} Li _{0.45} TiO ₃	5.01E-4		P4/mmm	123		50434	97
La _{0.565} Li _{0.305} TiO ₃	9.57E-4		P4/mmm	123		92235	59

$\text{La}_{0.58}\text{Li}_{0.27}\text{TiO}_3$	5.99E-4		P4/mmm	123		82672	97
$\text{Li}_4\text{PS}_4\text{l}$	1.2E-4	0.37	P4/nmmZ	129		432169	101
$\text{Li}(\text{LaTiO}_4)$	<1E-10	0.83	P4/nmmZ	129		91843	99
$\text{Li}(\text{NdTiO}_4)$	<1E-10	0.87	P4/nmmZ	129		91844	99
$\text{La}_{0.62}\text{Li}_{0.14}(\text{Mg}_{0.5}\text{W}_{0.5})\text{O}_3$	1.2E-5	0.37	P4/nmm	129		151902	100
$\text{La}_{0.63}\text{Li}_{0.11}(\text{Mg}_{0.5}\text{W}_{0.5})\text{O}_3$	6.8E-6	0.38	P4/nmm	129		151901	100
$\text{La}_{0.65}\text{Li}_{0.05}(\text{Mg}_{0.5}\text{W}_{0.5})\text{O}_3$	1.8E-7	0.46	P4/nmm	129		151900	100
Li_6ZnO_4	9.40E-09	0.61	P4 ₂ /nmc	137		62137	64
$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	3.98E-3	0.305	P4 ₂ /nmc	137		255750	108
$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	7E-3	0.27	P4 ₂ /nmc C	137		193755	107
$\text{Li}_{10}\text{GePS}_{12}$	1.21E-2		P4 ₂ /nmc	137		188887	104
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	1.20E-02	0.25	P4 ₂ /nmc	137		255749	110
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$	2.46E-2	0.274	P4 ₂ /nmc	137		241439	108
$\text{Li}_{10.35}\text{Ge}_{1.35}\text{P}_{1.65}\text{S}_{12}$	1.44E-2	0.269	P4 ₂ /nmc S	137		193947	104
$\text{Li}_{10.35}\text{Si}_{1.35}\text{P}_{1.65}\text{S}_{12}$	6.5E-3		P4 ₂ /nmcS	137		252037	109
$\text{Li}_{0.81}\text{Sn}_{0.81}\text{P}_{2.19}\text{S}_{12}$	5.5E-3		P4 ₂ /nmc	137		252040	109
$\text{Li}_{10}(\text{Ge}_{0.776}\text{Sn}_{0.224})\text{P}_2\text{S}_{12}$	1.41E-2	0.276	P4 ₂ /nmc	137		255748	108
$\text{Li}_{10.2}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.2}\text{P}_{1.8}\text{S}_{12}$	7.82E-3		P4 ₂ /nmcS	137		5667	111
$\text{Li}_{10.2}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.2}\text{P}_{1.8}\text{S}_{12}$	2.69E-3		P4 ₂ /nmcS	137		257948	111
$\text{Li}_{10.5}(\text{Sn}_{0.2}\text{Si}_{0.8})_{1.5}\text{P}_{1.5}\text{S}_{12}$	8.79E-3		P4 ₂ /nmcS	137		5668	111
$\text{LiLaNb}_2\text{O}_7$	<1E-8		I4/mmm	139		72566	114
$\text{Li}_4\text{Sr}_3\text{Nb}_6\text{O}_{20}$	<1E-10		I4/mmm	139		87824	115
$\text{Li}_4\text{Sr}_{3.056}\text{Nb}_6\text{O}_{20}$	<1E-10	0.74	I4/mmm	139		109168	115
$\text{Li}_4\text{Sr}_3\text{Nb}_{5.77}\text{Fe}_{0.23}\text{O}_{19.77}$	<1E-10		I4/mmm	139		87823	115

Li_3BN_2	8.70E-08	0.55	I4 ₁ /amd	141	$\beta\text{-Li}_3\text{BN}_2$	155126	93
LiScO_2	<1E-10	1.047	I4 ₁ /amd	141		257819	117
LiScO_2	1.00E-12	0.87	I4 ₁ /amd	141		36124	33
Li_4SrN_2	2.30E-13	0.9	I4 ₁ /amd	141		87413	116
LiAlO_2	1.10E-12	0.97	I4 ₁ /amd	141	r-LiAlO ₂	99517	33
$\text{Li}_{0.9}\text{Sc}_{0.9}\text{Zr}_{0.1}\text{O}_2$	<1E-10	0.912	I4 ₁ /amd	141		257820	117
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	1.63E-6	0.54	I4 ₁ /acdZ	142	"tetragonal-LLZO"	183684	119
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	9.9E-6	0.43	I4 ₁ /acdZ	142		238687	121
$\text{Li}_7\text{La}_3\text{HfO}_{12}$	9.85E-7	0.53	I4 ₁ /acdZ	142	"tetragonal-LLHO"	174202	118
LiAlGeO_4	<1E-10	0.97	R3H	146		257741	123
LiGaSiO_4	3.00E-16	0.9	R3H	146		65125	122
$\text{LiGa}_{0.5}\text{Al}_{0.5}\text{GeO}_4$	<1E-10	1.06	R3H	146		257740	123
LiGaGeO_4	<1E-10	1.12	R $\bar{3}$	148		257739	123
LiNaSO_4	8.80E-10		P31c	159		14364	125
$\text{Li}_4\text{P}_2\text{S}_6$	2.38E-07	0.29	P $\bar{3}1m$	162		242170	127
$\text{Li}_{2.667}\text{Mg}_{0.667}\text{P}_2\text{S}_6$	4.00E-06	0.46	P $\bar{3}1m$	162		95607	126
$\text{Li}_{3.333}\text{Mg}_{0.333}\text{P}_2\text{S}_6$	8.20E-8	0.517	P $\bar{3}1m$	162		95606	126
Li_3ErCl_6	3.3E-4	0.41	P $\bar{3}m1$	164		50151	129
Li_5NCl_2	1.20E-06	0.5	R $\bar{3}m$	166		84763	131
$\text{LiGe}_2(\text{PO}_4)_3$	3.33E-7		R $\bar{3}cH$	167		263767	2
$\text{LiGe}_2(\text{PO}_4)_3$	4.83E-9	0.654	R $\bar{3}cH$	167		69763	133
$\text{LiZr}_2(\text{PO}_4)_3$	2.96E-10		R $\bar{3}cH$	167		201935	2
$\text{LiTi}_2(\text{PO}_4)_3$	7.61E-6	0.38	R $\bar{3}cH$	167		95979	132

$\text{Li}(\text{Ti}_{0.4}\text{Sn}_{1.6})(\text{PO}_4)_3$	3.15E-6		R $\bar{3}$ cH	167		183677	135
$\text{Li}(\text{Ti}_{0.6}\text{Sn}_{1.4})(\text{PO}_4)_3$	9.42E-6		R $\bar{3}$ cH	167		183676	135
$\text{Li}(\text{Ti}_{1.4}\text{Sn}_{0.6})(\text{PO}_4)_3$	2.28E-5	0.32	R $\bar{3}$ cH	167		183672	135
$\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$	7E-4		R $\bar{3}$ cH	167		257190	139
$\text{Li}_{1.3}(\text{Al}_{0.3}\text{Ti}_{1.7})(\text{PO}_4)_3$	8.02E-7		R $\bar{3}$ cH	167		253240	138
$\text{Li}_{1.2}\text{Al}_{0.2}\text{Ge}_{1.8}(\text{PO}_4)_3$	4.83E-5	0.387	R $\bar{3}$ cH	167		263760	133
$\text{Li}_{1.3}(\text{Al}_{0.23}\text{Y}_{0.07}\text{Ti}_{1.7})(\text{PO}_4)_3$	3.84E-8		R $\bar{3}$ cH	167		253243	138
$\text{Li}_{1.3}(\text{Al}_{0.23}\text{Sc}_{0.07}\text{Ti}_{1.7})(\text{PO}_4)_3$	1.94E-7		R $\bar{3}$ cH	167		253242	138
$\text{Li}_{1.3}(\text{Al}_{0.23}\text{Ga}_{0.07}\text{Ti}_{1.7})(\text{PO}_4)_3$	4.46E-6		R $\bar{3}$ cH	167		253241	138
LiIO_3	1.90E-07		P6 ₃	173		35473	147
$\text{Li}_9\text{Mg}_3(\text{PO}_4)_4\text{F}_3$	<1E-10	0.835	P6 ₃	173		426103	148
$\text{Li}\text{Eu}_9\text{Si}_6\text{O}_{26}$	<1E-10		P6 ₃ /m	176		291220	150
$\text{Li}\text{La}_9\text{Si}_6\text{O}_{26}$	<1E-10		P6 ₃ /m	176		291218	150
$\text{Li}_{0.284}\text{Sm}_{4.512}\text{Si}_3\text{O}_{12.91}$	<1E-10		P6 ₃ /m	176		83279	150
$\text{Pb}_{6.12}\text{Ca}_{1.9}\text{Li}_{1.96}(\text{PO}_4)_6$	<1E-10	1.05	P6 ₃ /m	176		59615	149
$\text{Li}_3(\text{NH}_2)_2\text{I}$	1E-5	0.58	P6 ₃ mc	186		167528	152
$\text{Ba}_3\text{LiTa}_5\text{ZrSi}_4\text{O}_{26}$	<1E-10	0.79	P6 ₂ m	189		239277	153
Li_3N	1.2E-3	0.25	P6/mmm	191		26540	154
Li_3N	3.00E-04	0.26	P6/mmm	191		156894	155
$\text{Fe}_2\text{Na}_2\text{K}(\text{Li}_3\text{Si}_{12}\text{O}_{30})$	<1E-10	1.22	P6/mcc	192		235750	156
Li_3P	7.03E-4	0.18	P6 ₃ /mmc	194		642223	157
$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	8E-6	0.43	I2 ₁ 3	199		54865	159
$(\text{K}_{0.1}\text{Li}_{0.9})(\text{SbO}_3)$	1.36E-8		Pn $\bar{3}$ Z	201		200984	160
Li_8SiP_4	4.5E-5	0.404	Pa $\bar{3}$	205		235186	161

Li_8GeP_4	1.8E-5	0.435	$\text{Pa}\bar{3}$	205	$\alpha\text{-Li}_8\text{GeP}_4$	235184	161
Li_3AlN_2	5.00E-08	0.45	$\text{Ia}\bar{3}$	206		257464	162
$\text{Li}_2\text{ZnGe}_3\text{O}_8$	<1E-10	2.14	$\text{P}4_3\text{2}$	212		86169	163
$\text{Li}_2\text{MgTi}_3\text{O}_8$	<1E-10	0.71	$\text{P}4_3\text{2}$	212		86165	163
$\text{Li}_2\text{CoTi}_3\text{O}_8$	<1E-10	1.33	$\text{P}4_3\text{2}$	212		86166	163
$(\text{Li}_{0.55}\text{Mg}_{0.45})(\text{Li}_{0.445}\text{Mg}_{0.055})\text{Ti}_{1.5}\text{O}_4$	1.53E-11	0.786	$\text{P}4_3\text{2}$	212		168145	164
$(\text{Li}_{0.61}\text{Mg}_{0.39})(\text{Li}_{0.46}\text{Mg}_{0.005})\text{Ti}_{1.5}\text{O}_4$	6.56E-10	0.685	$\text{P}4_3\text{2}$	212		168144	164
Li_2VCl_4	6.95E-6		$\text{F}\bar{4}3\text{m}$	216		74959	166
Li_5NI_2	4.00E-6		$\text{F}\bar{4}3\text{m}$	216		16800	165
$\text{Li}_6\text{PO}_5\text{Cl}$	5.54E-10	0.66	$\text{F}\bar{4}3\text{m}$	216		421479	173
$\text{LiCe}(\text{BH}_4)_3\text{Cl}$	1.03E-4		$\text{I}\bar{4}3\text{m}$	217		185218	178
Li_7PN_4	1.60E-07	0.4	$\text{P}\bar{4}3\text{n}$	218		69017	95
$\text{Li}_4\text{B}_7\text{O}_{12}\text{Cl}$	2.4E-5		$\text{F}\bar{4}3\text{c}$	219		1125	179
Li_9NS_3	8.30E-07	0.52	$\text{Pm}\bar{3}\text{m}$	221		240749	185
Li_3OBr	1.10E-06	0.74	$\text{Pm}\bar{3}\text{m}$	221		67265	194,195
$\text{Li}_2(\text{OH})\text{Br}$	1.20E-6	0.75	$\text{Pm}\bar{3}\text{m}$	221		200874	184
$(\text{La}_{0.55}\text{Li}_{0.45})(\text{Ti}_{0.9}\text{Al}_{0.1})\text{O}_3$	1.51E-3		$\text{Pm}\bar{3}\text{m}$	221		254045	186
$(\text{La}_{0.6}\text{Li}_{0.4})(\text{Ti}_{0.8}\text{Al}_{0.2})\text{O}_3$	5.68E-4		$\text{Pm}\bar{3}\text{m}$	221		254046	186
$(\text{La}_{0.65}\text{Li}_{0.35})(\text{Ti}_{0.7}\text{Al}_{0.3})\text{O}_3$	1.61E-4		$\text{Pm}\bar{3}\text{m}$	221		254047	186
$(\text{La}_{0.402}\text{Li}_{0.368}\text{Sr}_{0.230})(\text{TiO}_3)$	2.87E-5	0.36	$\text{Pm}\bar{3}\text{m}$	221		190827	183
$(\text{La}_{0.46}\text{Li}_{0.429}\text{Sr}_{0.111})(\text{TiO}_3)$	1.97E-4	0.33	$\text{Pm}\bar{3}\text{m}$	221		190826	183
$(\text{La}_{0.49}\text{Li}_{0.461}\text{Sr}_{0.049})(\text{TiO}_3)$	7.09E-4	0.33	$\text{Pm}\bar{3}\text{m}$	221		190825	183

$(\text{Li}_{0.16}\text{Sr}_{0.69})(\text{Ga}_{0.25}\text{Ta}_{0.75})\text{O}_3$	3.69E-6	0.359	Pm $\bar{3}$ m	221		291520	187
$\text{Li}_{0.31}\text{La}_{0.63}((\text{Ti}_{0.9}\text{Co}_{0.1})\text{O}_3$	2.60E-4		Pm $\bar{3}$ m	221		151533	182
Lil	1E-7		Fm $\bar{3}$ m	225		414244	197
$\text{Li}_{7.2}\text{N}_{1.6}\text{Cl}_{2.4}$	8.4E-7	0.49	Fm $\bar{3}$ m	225		49646	131
$\text{Li}_{0.19}\text{La}_{0.67}(\text{Ti}_{0.9}\text{Co}_{0.1})\text{O}_3$	1.08E-4		Fm $\bar{3}$ m	225		151535	182
LiCdCl_4	5.80E-07	0.44	Fd $\bar{3}$ m	227		74958	199
Li_2MgCl_4	6.24E-7		Fd $\bar{3}$ m	227		74957	166
Li_2MnCl_4	4.79E-6		Fd $\bar{3}$ m	227		69678	166
$\text{Li}(\text{Li}_{0.34}\text{Ti}_{1.66})\text{O}_4$	6.03E-8	0.506	Fd $\bar{3}$ m	227		168137	164
$\text{Li}_{1.9}\text{Mn}_{0.9}\text{Ga}_{0.1}\text{Cl}_4$	2.37E-7		Fd $\bar{3}$ m	227		50305	198
$(\text{Li}_{0.74}\text{Mg}_{0.26})(\text{Li}_{0.40}\text{Mg}_{0.04}\text{Ti}_{1.56})\text{O}_4$	1.51E-9	0.639	Fd $\bar{3}$ m	227		168142	164
$(\text{Li}_{0.826}\text{Mg}_{0.174})(\text{Li}_{0.374}\text{Mg}_{0.026}\text{Ti}_{1.60})\text{O}_4$	4.24E-9	0.615	Fd $\bar{3}$ m	227		168141	164
$\text{LiSrTa}_2\text{O}_6\text{F}$	<1E-10	0.604	Fd $\bar{3}$ m	227		236010	200

IV. W_σ optimization

Ward's minimum variance method applied to the conductivity labels (W_σ) is used to assess the utility of each descriptor-simplification combination. The W_σ is calculated after agglomerative clustering, for each clustering set:

$$W_\sigma = \sum_{k=1}^{n_c} \sum_{i \in C_k} [\log(\sigma_{RT})_i - \overline{\log(\sigma_{RT})}_k]^2$$

where n_c is the number of clusters in a set, C_k is cluster k , and where $\overline{\log(\sigma_{RT})}_k$ denotes the mean for all labels in cluster k . Lower W_σ values indicate that the descriptor-simplification combination results in clustering where structures with similar conductivity are grouped together. Whereas a large W_σ indicates that the clusters have little correlation to the conductivity labels.

A frozen-state strategy is employed to prevent any label from dropping out of the W_σ calculation. The frozen-state strategy operates by calculating the partial variance (PV) for each label at each clustering depth:

$$PV_{x,C_k} = [\log(\sigma_{RT})_x - \overline{\log(\sigma_{RT})}_k]^2$$

where PV_{x,C_k} is the partial variance for label x , when label x is assigned to cluster k . The PV for each label is saved before summing all the partial variances to yield the W_σ . At each subsequent clustering depth, all new clusters are checked to determine whether any cluster contains a single label. If a label is the only label in a cluster, then that label's partial variance is frozen: its PV_{x,C_k} becomes equal to the saved state from the previous cluster depth:

$$PV_{x,C_j} = PV_{x,C_k}$$

where C_j denotes the cluster with only one label and C_k denotes the cluster that label x previously resided in. Without the frozen state strategy, poor models will reach desirable W_σ values at sufficient depths of clustering. The artificial depression of the W_σ value occurs because clusters that contain a single label evaluate to 0 (the label mean and cluster mean are the same). Whereas the frozen state strategy effectively “remembers” how well (or poorly) the label was clustered before it drops out.

Hyperparameter tuning was employed for some of the descriptors. At least one W_σ representation exists for each unique combination of structure simplification and descriptor. However, some of the descriptors can be altered by tuning associated hyperparameters, resulting in more W_σ representations. The descriptors with hyperparameter tuning are the global instability index, radial distribution function, smooth overlap of atomic positions (SOAP), and mXRD. A grid search was done over the hyperparameters, for each descriptor, with parameters shown in table S1.

Descriptor	Hyper-parameter	Description	Values attempted in grid search
Global instability index	r_cut	The distance, in angstroms, to search for neighbors when calculating bond valences.	[1.0, 1.1, ..., 5.9, 6.0]

Radial distribution function	cutoff	The distance, in angstroms, over which the radial distribution function should be calculated.	[1, 2, ..., 29, 30]
	bin_size	The radial distance, in angstroms, for each bin.	[0.01, 0.02, ..., 0.09, 0.1, 0.2, ..., 0.9, 1.0]
Smooth overlap of atomic positions (SOAP)	rcut	The radial cutoff for the local region in angstroms.	[1, 2, ..., 29, 30]
	nmax	The number of radial basis functions used.	[2, 3, ..., 8, 9]
	lmax	The maximum degree of spherical harmonics used.	[1, 2, ..., 8, 9]
	average	The averaging mode.	['outer', 'inner']
mXRD	pattern_length	The number of 2θ values that will be calculated between 0° and 90° .	[101, 201, ..., 901, 1001]

Ultimately, the SOAP-CAN descriptor-simplification outperforms all other descriptor-simplifications when the averaging hyperparameter is set to ‘outer’. Setting the ‘outer’ hyperparameter results in averaging over the power spectrum of different sites. Whereas the ‘inner’ setting averages over the sites first, before summing up the magnetic quantum numbers. The other three hyperparameters (rcut, nmax, and lmax) are less consequential, with most combinations tested outperforming all other non-SOAP descriptors. To illustrate the point, three different SOAP–CAN outcomes are depicted in Figure S1, plotted against the best-performing outcomes from density-CAN, mXRD-A40, orbital field matrix, and structure heterogeneity-A40. The three SOAP-CAN outcomes are those with the lowest W_σ mean for the depth of clustering ranges: 2-100, 101-200, and 201-300. The respective hyperparameters for the three SOAP-CAN descriptors are [rcut=2, nmax=4, lmax=2], [rcut=4, nmax=2, lmax=2], and [rcut=3, nmax=5, lmax=3].

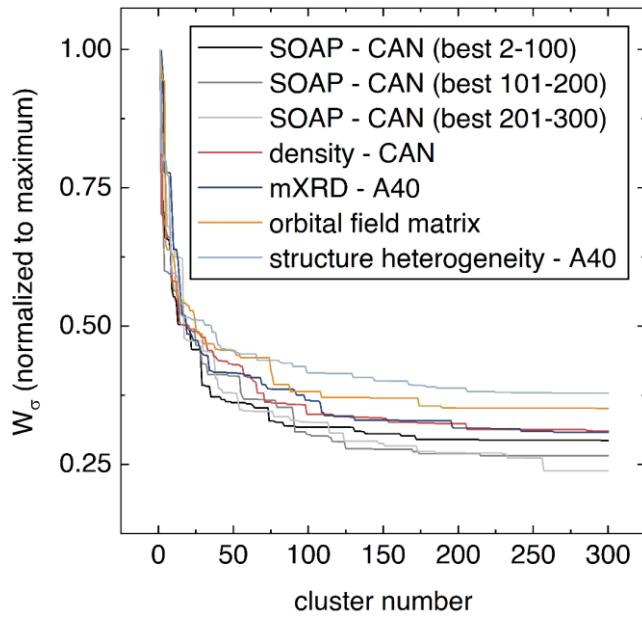


Figure S1. W_σ vs. cluster number for three different SOAP-CAN models compared with the best-performing models for density-CAN, mXRD-A40, orbital field matrix, and structure heterogeneity-A40. The three SOAP-CAN models are those with the lowest W_σ mean for the clustering ranges: 2-100, 101-200, and 201-300. Almost all SOAP-CAN models outperformed the best non-SOAP models, irrespective of the specific combination of $rcut$, $nmax$, and $lmax$ hyperparameters.

V. W_{Ea} optimization

Each clustering outcome is also assessed by labeling with approximate activation energies for ion hopping. The activation energies are calculated using a bond valence site energy (BVSE) method developed by Adams and Rao^{331,332}. The strategy approximates the E_a as the sum of an attractive Morse-type potential term and a repulsive Coulombic interaction term. The Morse-type potential term represents mobile ion interactions with lattice anions. While the Coulombic interaction term represents mobile ion interactions with lattice cations. Relative to DFT-based methods, the BVSE method is a computationally lean approach that can be used to readily assess thousands of structures. However, the BVSE method tends to overestimate activation energies because it (1) does not allow for structural relaxation as the mobile ion moves and (2) does not consider repulsive interactions between mobile ions^{331,332}. The BVSE method has been implemented by He et al. and is available for use through their python API³³³. Using the BVSE method, we label 6845 structures with activation energies (6845 is the number of structures successfully solved given a computing time cutoff of 20-minutes for each structure). Ward's minimum variance method applied to the activation energy labels (W_{Ea}) is calculated in a similar manner to the W_σ :

$$W_{Ea} = \sum_{k=1}^{n_c} \sum_{i \in C_k} \left[(E_{a,BVSE})_i - (\overline{E_{a,BVSE}})_k \right]^2$$

where n_c is the number of clusters in a set, C_k is cluster k , and where $(\overline{E_{a,BVSE}})_k$ denotes the mean for all labels in cluster k . Each descriptor's W_{Ea} results are shown in Figure S2 for the first 50 clustering sets. For simplicity, only the best-performing simplification-descriptor combination is shown for each descriptor.

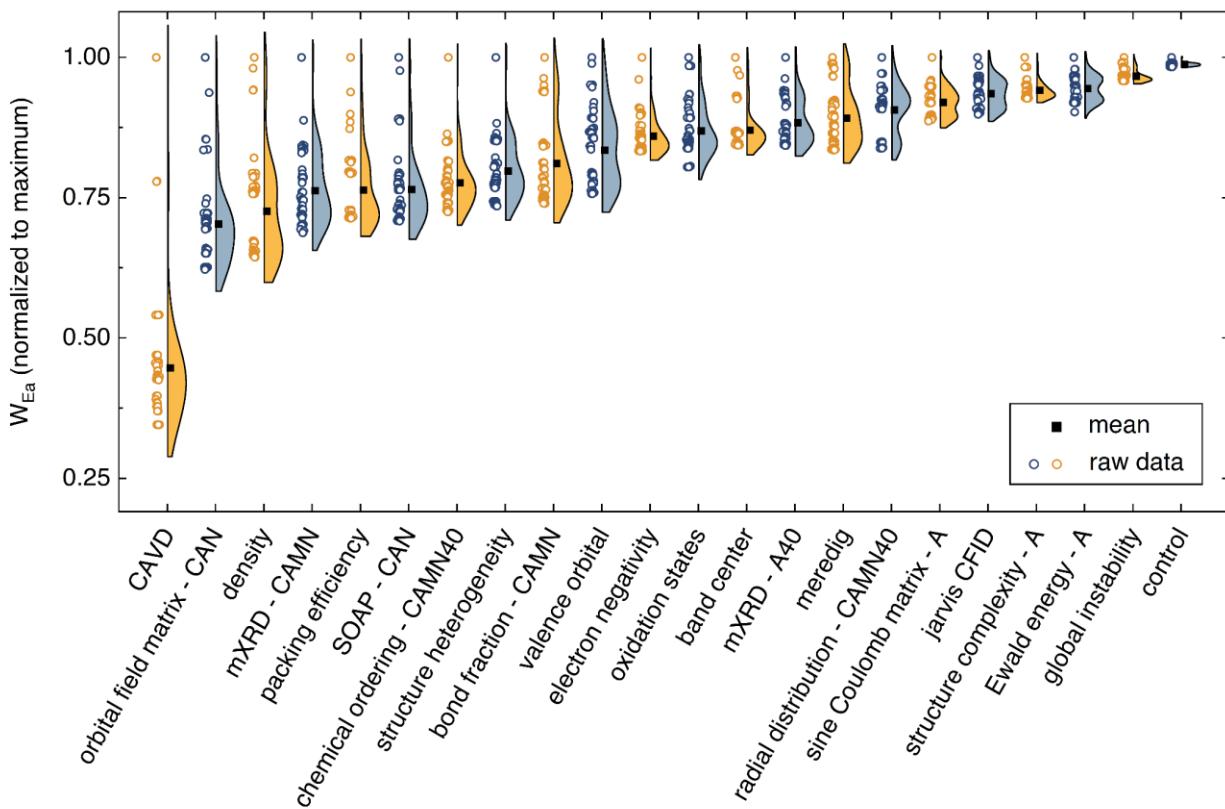


Figure S2. The W_{E_a} for the first 50 clusters generated using each descriptor. Half-violin plots show the raw W_{E_a} score for each cluster as symbols next to the violin distribution. Simplification-descriptor combinations are sorted in order of ascending mean. The control is a random assignment of clusters, with W_{E_a} values averaged over 100 randomly assigned sets.

For E_a labels, all descriptor-simplification pairings result in better semi-supervised ML performance than randomized clustering. The SOAP descriptor performs well relative to most, but five other descriptors outperform it: CAVD, orbital field matrix-CAN, density, mXRD-CAMN, and the packing efficiency descriptors. The favorable performance of CAVD is anticipated because the BVSE calculation directly uses the CAVD descriptor as a parameter. The favorable performance of the density and packing efficiency descriptors may be explained by their similarity to CAVD: the Voronoi decomposition to encode void space is dependent on the density and packing efficiency of the structure. Similarly, the orbital field matrix descriptor relies on calculation of Voronoi polyhedra to understand the coordination environment for each atom. A mXRD-CAMN descriptor-simplification performs well on the BVSE label set; however, the mXRD representation used by Toyota (mXRD – A40) drops from to 14th best on the E_a label set. The result may suggest that the mXRD – A40 pairing does not generalize well. When comparing the top 10 descriptors for each label set, 6 descriptors are common to both approaches: SOAP, density, mXRD, structure heterogeneity, orbital field matrix, and bond fraction.

VI. Second-order SOAP descriptor

Semi-supervised ML models may be further improved by merging descriptors and clustering on the union representation. Second order descriptor unions are examined by combining the best-performing descriptors with all other descriptors. The two input descriptor vectors (d_A and d_B) were combined with a mixing ratio (α) to yield the union representation (d_{AB}):

$$d_{AB} = d_A \cup \alpha d_B$$

The ideal mixing ratio is unknown for each union and we find that incremental changes to the mixing ratio do not result in continuous changes to the W_σ . Thus, outcomes are manually screened for mixing ratios from 10^{-6} to 10^6 (see supplemental information – section VI). Most descriptor unions result in no improvement to the W_σ , across all mixing ratios. However, the W_σ for SOAP when mixing with the non-simplified sine Coulomb matrix descriptor (for $\alpha = 2 \cdot 10^{-6}$ - $4 \cdot 10^{-6}$) is lowered by 2-3%, with the exact percentage depending on the depth of clustering.

Almost no descriptor combinations are successful in reducing the W_σ . Excluding combinations that include the SOAP-CAN descriptor, no combinations outperform the 1st order SOAP-CAN representation. For combinations that include SOAP-CAN, some mixing ratios with the sine Coulomb matrix and the Ewald energy descriptors resulted in modest improvements in the W_σ . The best improvement is found when mixing SOAP-CAN with the sine Coulomb descriptor for $\alpha = 2 \cdot 10^{-6}$, $3 \cdot 10^{-6}$, and $4 \cdot 10^{-6}$. All three combinations result in the same improved curve, plotted below in Figure S3.

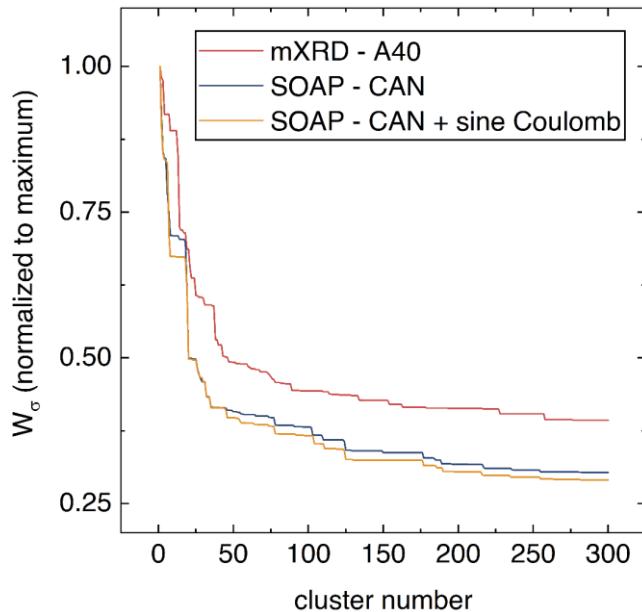


Figure S3. The best performing 2nd order descriptor: SOAP-CAN mixed with the sine Coulomb descriptor. The clustering performance is shown for the full label set of 219. Since the mXRD – A40 representation is also compatible with the full label set, it is shown for reference. The 2nd order descriptor outperforms the 1st order SOAP-CAN descriptor at most depths of clustering.

The agglomerative dendrogram in the main text shows that the 2nd-order SOAP-CAN descriptor facilitates aggregation of high-conductivity labels. In the simplified 9-cluster representation, most of the high-conductivity ($\sigma_{RT} > 10^{-5}$ S cm⁻¹) labels are contained within the 2nd

“mega cluster”. The 2nd mega cluster accounts for only 15% of the input structure. By clustering further, increasingly dense representations are found. For example, at the 241st clustering depth, the 21 high-conductivity labels have been sorted into five subclusters (Figure S4). Taken together, the five subclusters account for 52.5% of the high conductivity labels while containing only 2.2% of the input structures. We note that the control (random clustering) exhibits a Ward Variance 214% greater than the 2nd-order SOAP-CAN model at the 241st clustering depth. The difference in Ward Variance illustrates that the 2nd-order SOAP-CAN model is much better at identifying high-conductivity structures, relative to random selection.

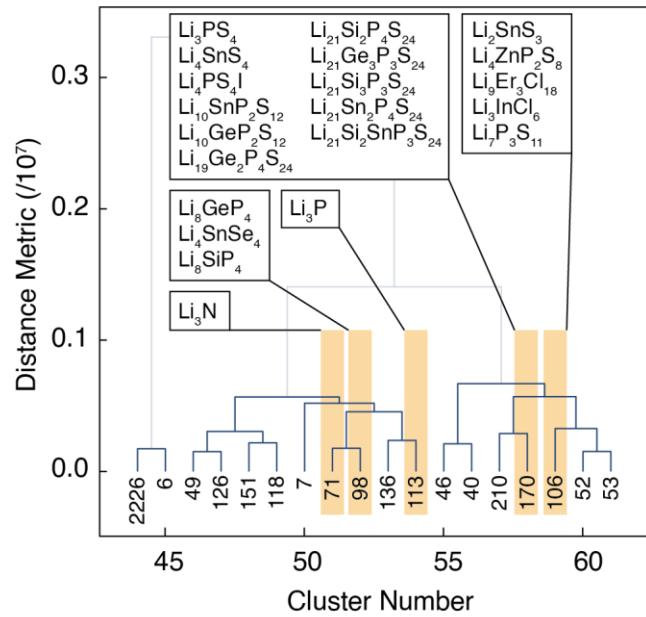


Figure S4. The partial agglomerative dendrogram generated for the 2nd-order SOAP-CAN descriptor-simplification. The area shown is the 2nd mega cluster taken from Figure 3 of the main text. At a clustering depth of 241, the 21 high-conductivity labels are sorted into 5 clusters which account for 2.2% of the input structures.

VII. Climbing Image – Nudged Elastic Band

Migration barriers for Li ion hopping are evaluated with the Climbing Image – Nudged Elastic Band (CI-NEB) method as implemented in the QuantumESPRESSO PWneb software package^{334–337}. Density-functional theory (DFT) calculations are performed using the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation functional and projector-augmented wave (PAW) sets^{338,339}. Convergence testing for the kinetic-energy cutoff of the plane-wave basis and the k -point sampling is performed for each structure to ensure an accuracy of 1 meV per atom. The lattice parameters and atomic positions of the as-retrieved structure are optimized. Supercells are created for each structure that are a minimum of 10 Å in each lattice direction to minimize interactions between periodic images of the mobile ion. To study the migration barrier in the dilute limit, a single Li vacancy is created in the boundary endpoint structures of each studied pathway. A uniform background charge is used to balance excess charge. Each boundary configuration is relaxed until the force on each atom is less than 3×10^{-4} eV/Å. Images are created by linearly interpolating framework atomic positions between the initial and final boundary configurations. The initial pathway for the mobile ion is generated from the BVSE output minimum energy pathway to promote faster convergence of the NEB calculation. An NEB force convergence threshold of 0.05 eV/ Å is used. The calculation is first converged using the default NEB algorithm and then restarted with the CI scheme to allow for the maximum energy of the pathway to be determined.

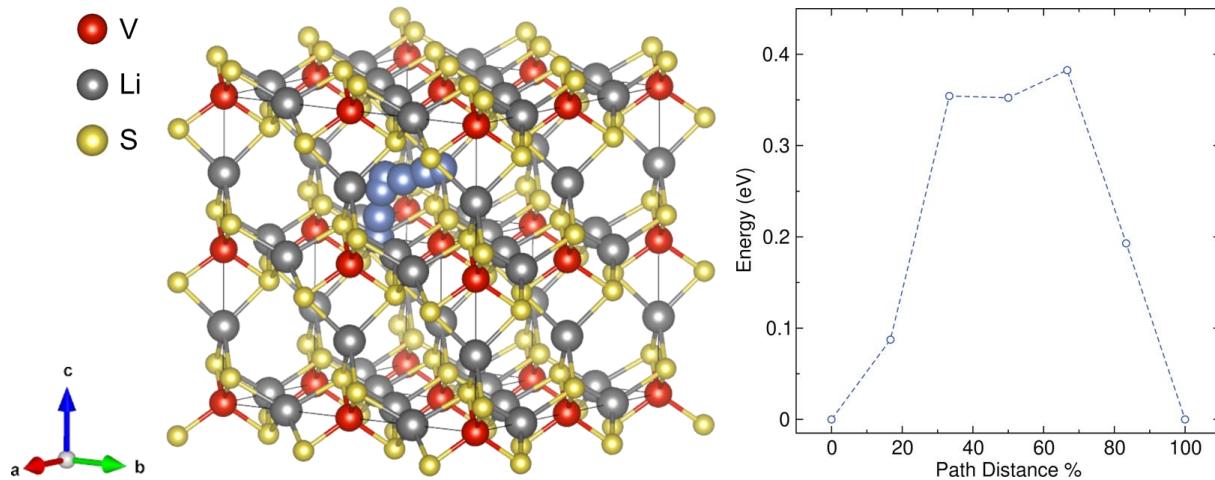


Figure S5. The 2x2x2 supercell of Li_3VS_4 used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

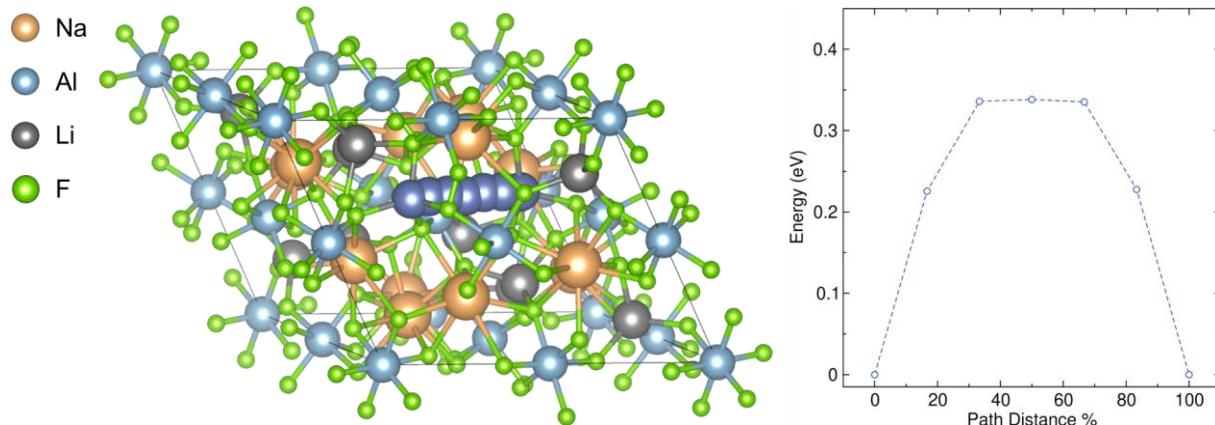


Figure S6. The primitive cell of $\text{Na}_3\text{Li}_3\text{Al}_2\text{F}_{12}$ used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

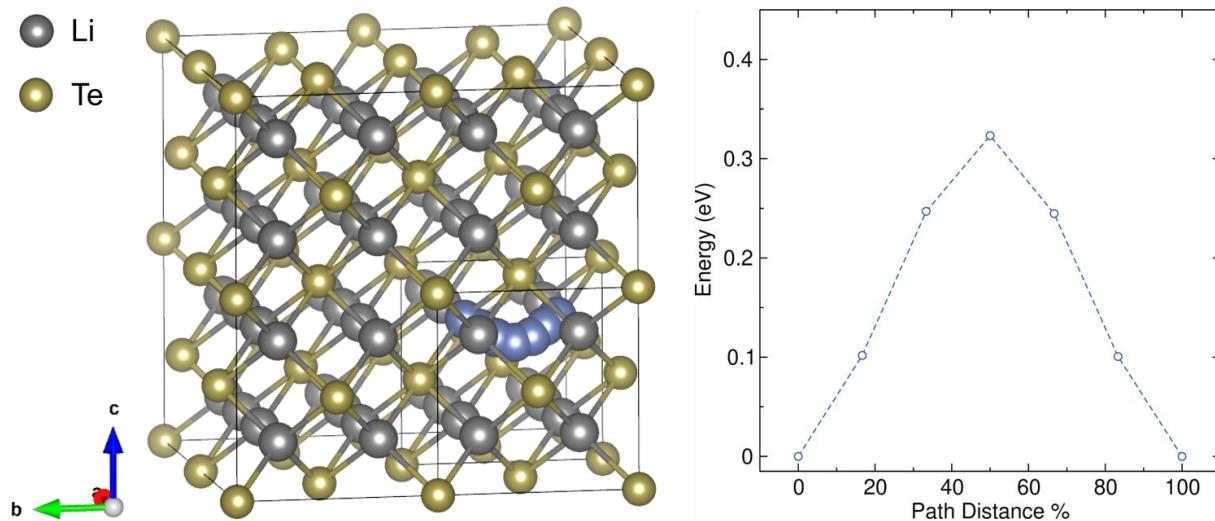


Figure S7. The $2 \times 2 \times 2$ supercell of Li_2Te used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

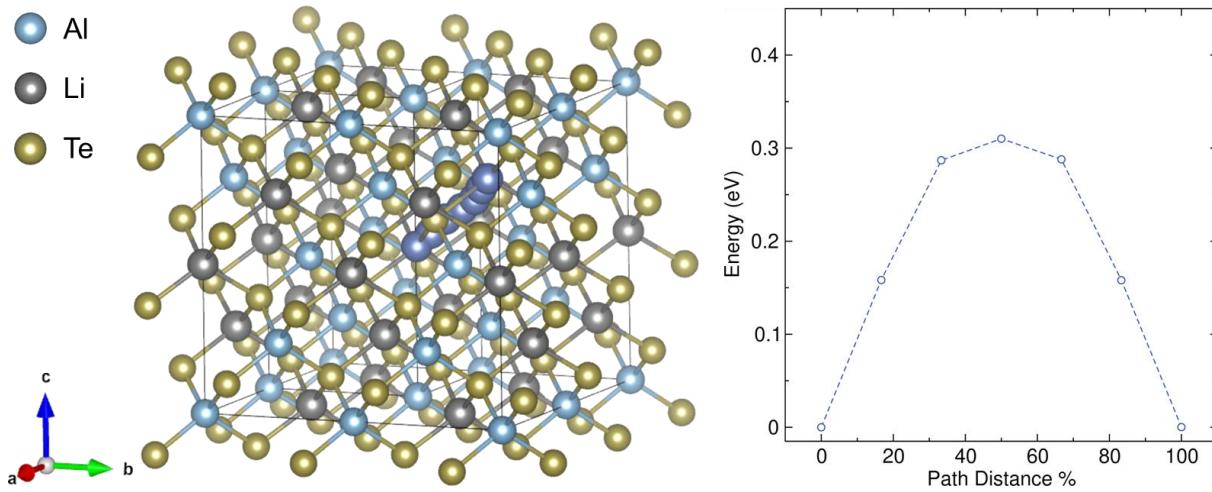


Figure S8. The 2x2x1 supercell of LiAlTe_2 used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

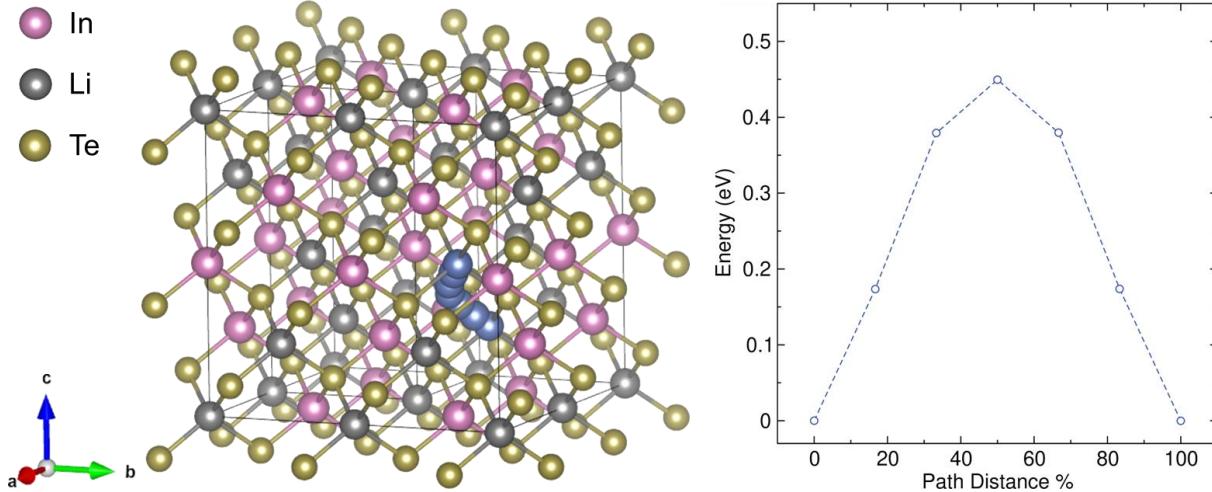


Figure S9. The 2x2x1 supercell of LiInTe_2 used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

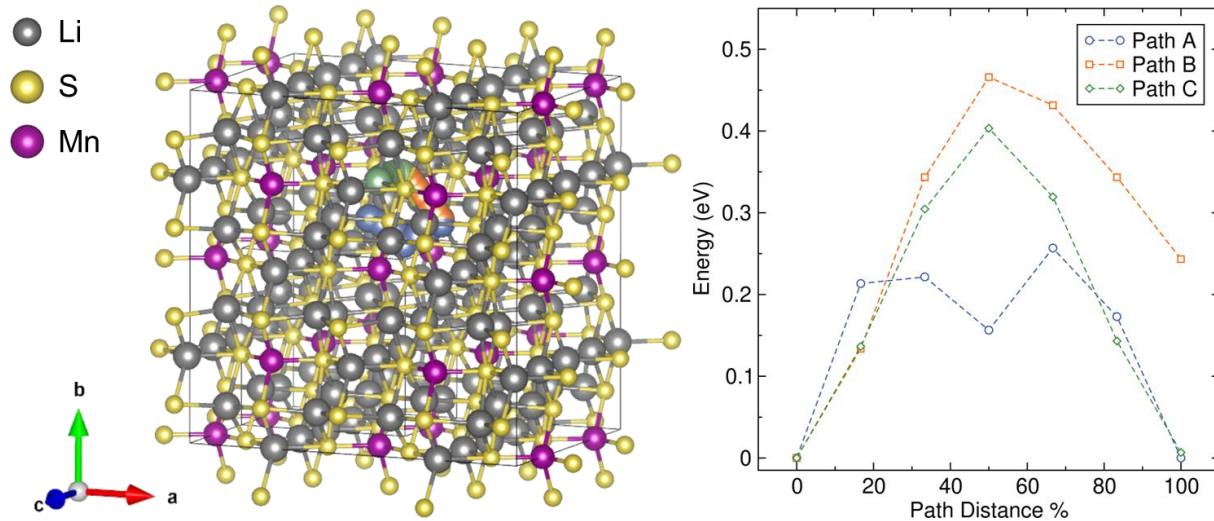


Figure S10. The $2 \times 2 \times 2$ supercell of Li_6MnS_4 used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

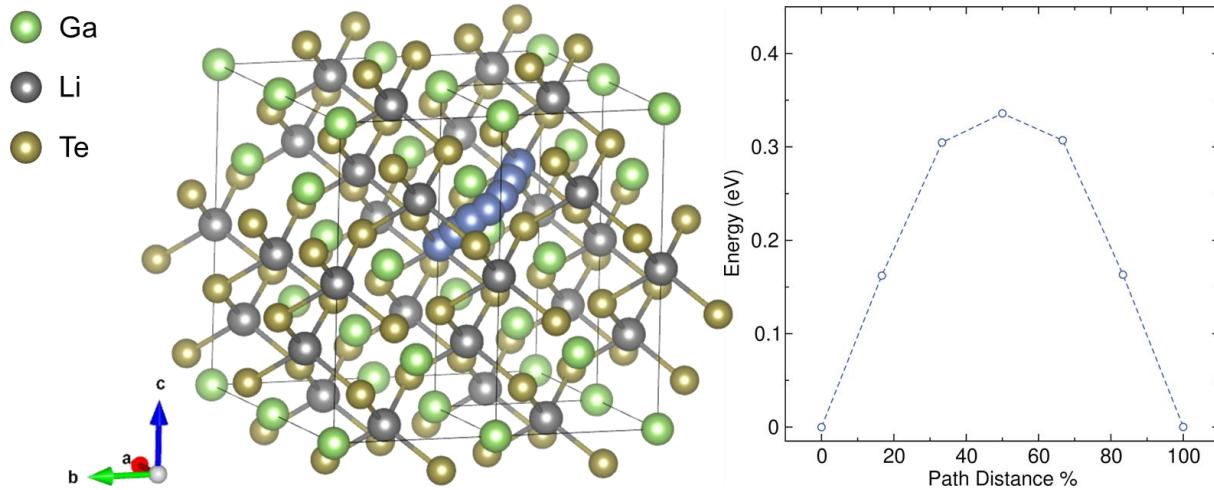


Figure S11. The $2 \times 2 \times 1$ supercell of LiGaTe_2 used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

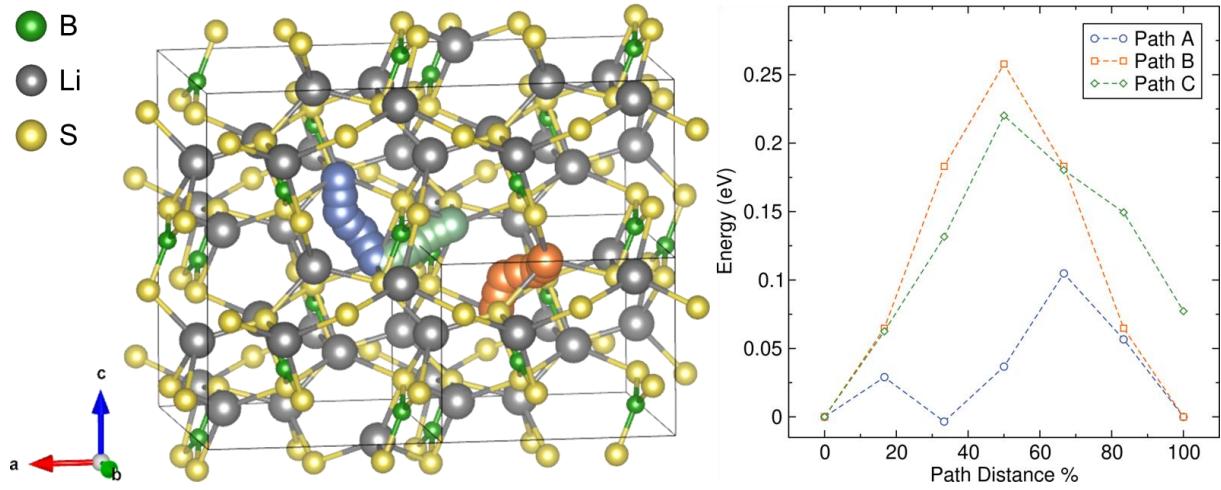


Figure S12. The 2x1x2 supercell of Li_3BS_3 used for the CI-NEB calculation of Li migration energy. Blue, green, and orange atoms represent the Li position from the CI-NEB output images.

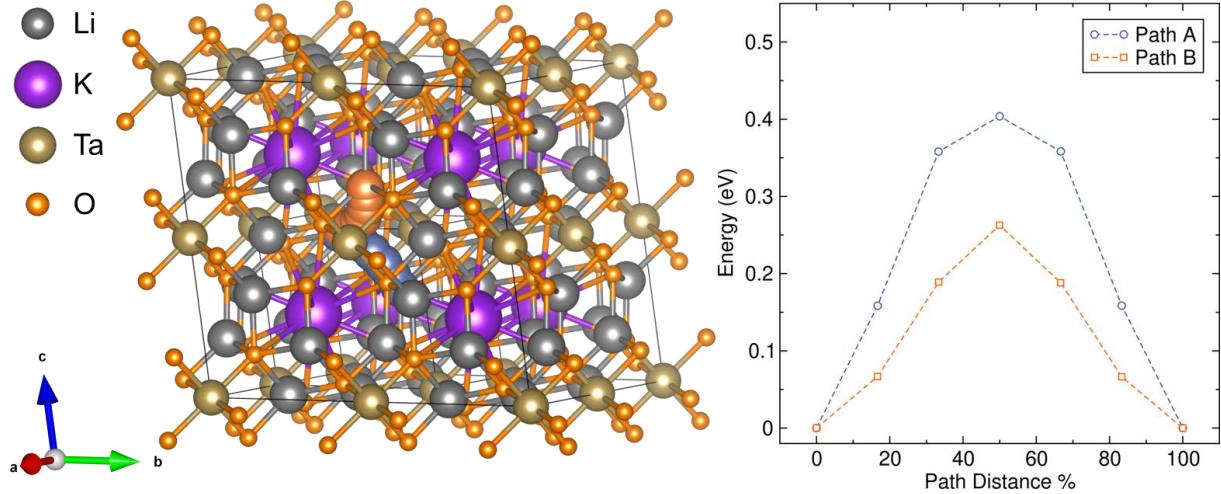


Figure S13. The 2x2x2 supercell of KLi_6TaO_6 used for the CI-NEB calculation of Li migration energy. Blue and orange atoms represent the Li position from the CI-NEB output images.

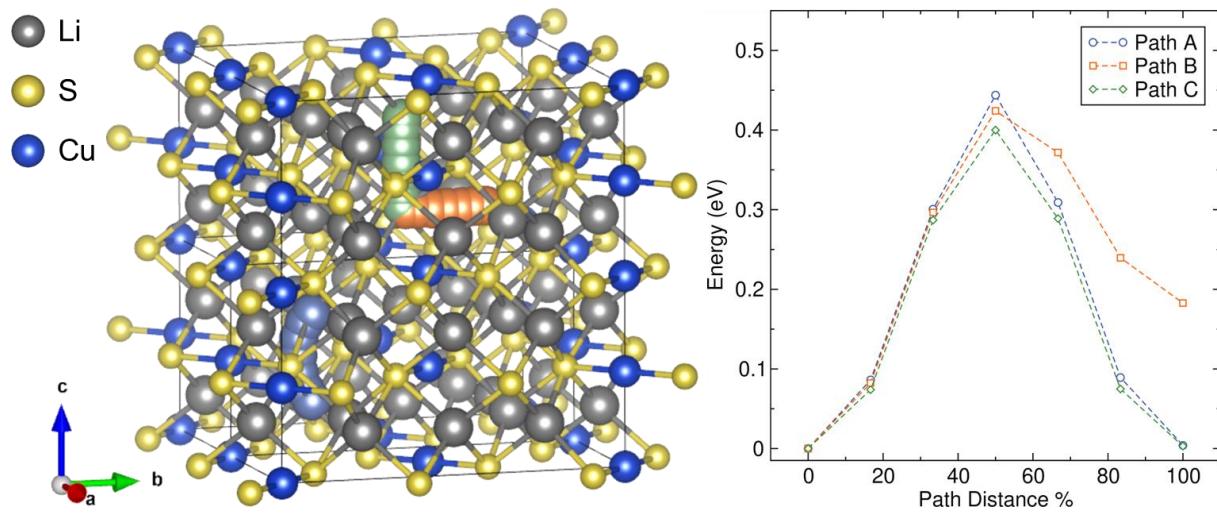


Figure S14. The 2x1x2 supercell of Li_3CuS_2 used for the CI-NEB calculation of Li migration energy. Blue atoms represent the Li position from the CI-NEB output images.

VIII. a-Li_{2.95}B_{0.95}Si_{0.05}S₃ impedance

Electrochemical impedance data for the amorphized Si-substituted Li₃BS₃ (a-Li_{2.95}B_{0.95}Si_{0.05}S₃) suggests the presence of two RC features. The VSP-300 potentiostat can supply a maximum sinusoidal frequency of 3 MHz, sufficient to resolve a partial semicircle in the Nyquist impedance plot (Figure S14). Attempted fits to the partial semicircle reveal that it would not intersect the origin at higher frequencies, suggesting the presence of an additional RC feature. It is plausible that two RC features exist, describing the bulk and grain-boundary transport of Li⁺. A more conservative estimate of the conductivity (σ_{tot}) can be derived by extrapolating a linear of the Warburg tail to the x intercept. While the more conservative estimate is used in the main manuscript, we note here that the actual bulk conductivity is likely higher.

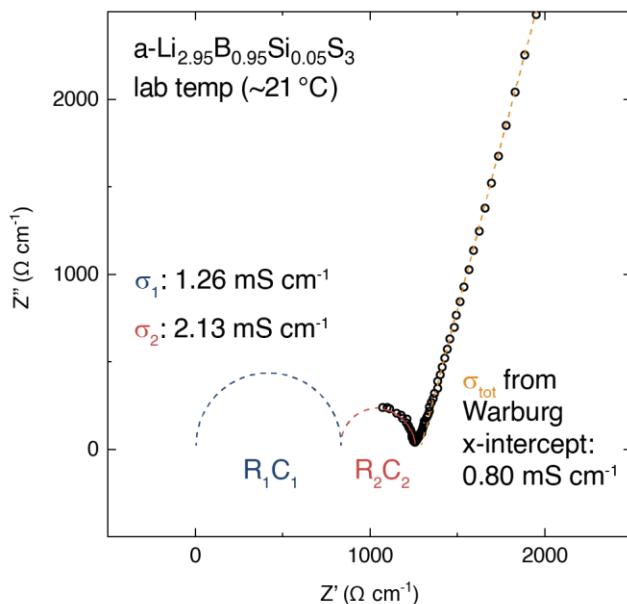


Figure S15. Nyquist data for a-Li_{2.95}B_{0.95}Si_{0.05}S₃ near room temperature. The partially resolved semi-circular features suggests the presence of at least two RC circuit elements.

IX. Full list of promising structures

Excluding the labeled dataset, there are 50 compounds that are predicted to be stable and to exhibit a Li-hopping activation energy below 600 meV. Ten of the predicted compounds have already been experimentally examined and are hereafter excluded: Li_2O , Li_2S , LiCl , LiI , LiBr , $\text{Li}_6\text{AsS}_5\text{I}$, $\text{Li}_4\text{Ti}_5\text{O}_{12}$, Li_2InCl_3 , LiInI_4 , Li_6NiCl_8 . Another nine are excluded because they are used in cathodes, anodes, or glassy electrolyte formulations: LiFeCl_4 , Li_2CO_3 , Li_2PtO_3 , $\text{Li}_2\text{NiGe}_3\text{O}_8$, Li_2CrO_4 , Li_2SeO_4 , LiAlS , $\text{Li}_2\text{Mn}_3\text{NiO}_8$, LiInSe_2 . The remaining 31 promising structures are discussed below and plotted by ascending activation energy in Figure S15.

a. Stable compounds

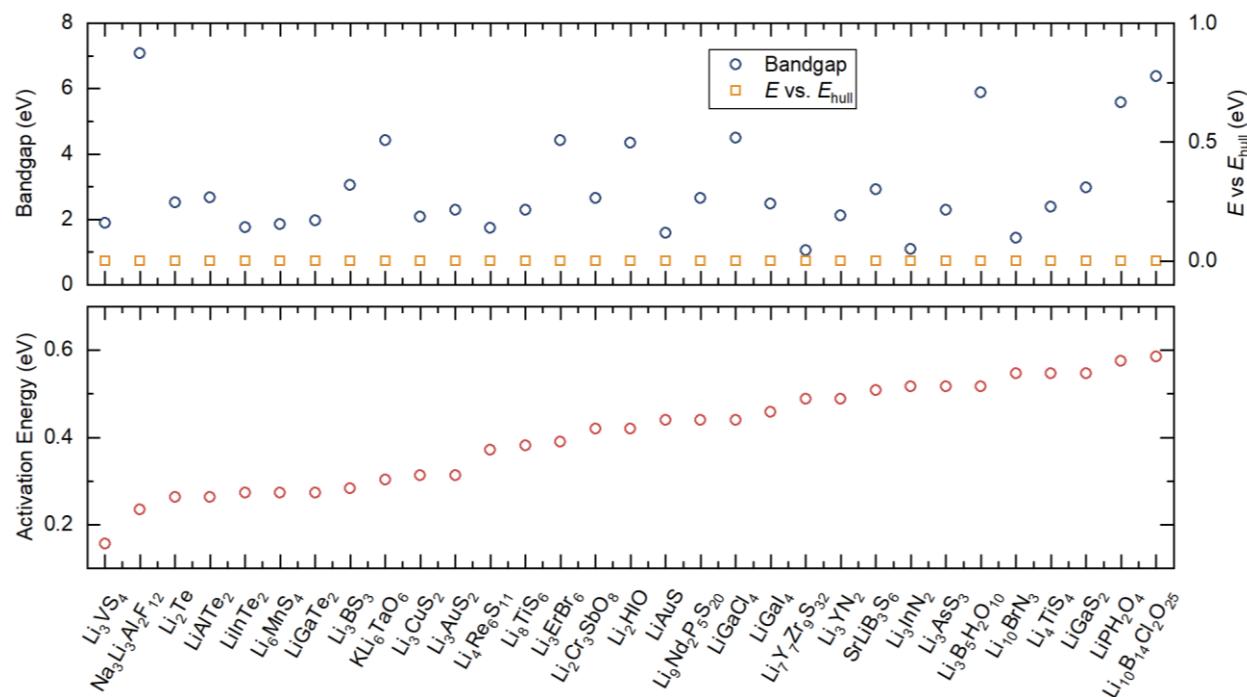


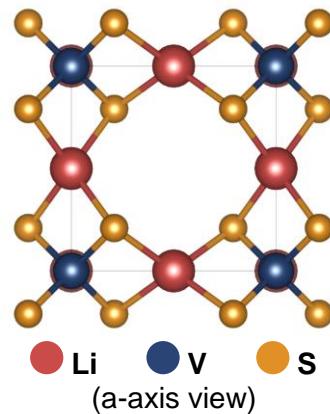
Figure S16. The 31 promising structures that are predicted to be stable and to exhibit Li-hopping activation energy below 600 meV.

Each structure is examined in order of ascending activation energy below.

Li_3VS_4

Material's Project ID	mp-760375
ICSD ID	None
Space Group	$P\bar{4}3m$ [215]
Calculated Band Gap	1.8951 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	156.25 meV

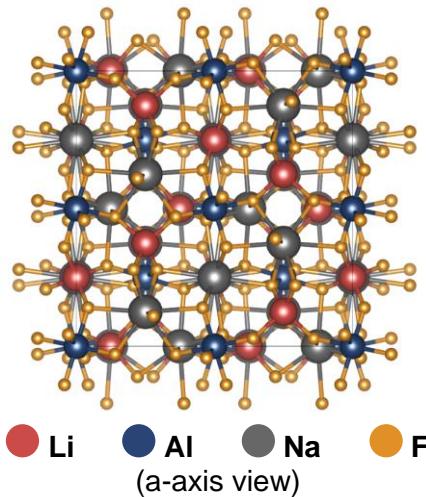
Notes: Explored for use as both an anode³⁴⁰ and a cathode³⁴¹. NEB has been employed to predict an activation energy of 95 meV.³⁴² All Li occupies tetrahedral sites that are edge sharing with adjacent V tetrahedra.



$\text{Na}_3\text{Li}_3\text{Al}_2\text{F}_{12}$

Material's Project ID	mp-6711
ICSD ID	9923
Space Group	$Ia\bar{3}d$ [230]
Calculated Band Gap	7.0872 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	234.38 meV

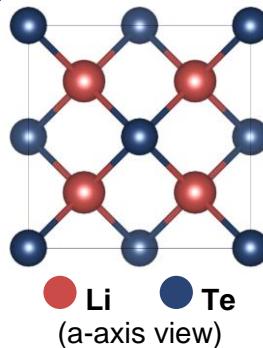
Notes: The structure appears to be unexplored. Discussion of structural motifs by Geller et al.³⁴³ All Li atoms are in a tetrahedral bonding environment.



Li_2Te

Material's Project ID	mp-2530
ICSD ID	60434
Space Group	$Fm\bar{3}m$ [225]
Calculated Band Gap	2.5171 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	263.67 meV

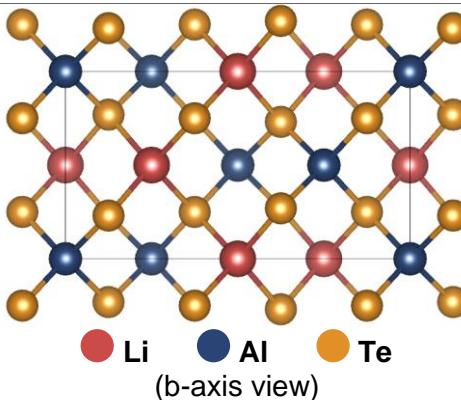
Notes: A screening approach using bond valence site energy calculations identified the oxide as a promising structure: $\text{Li}_2\text{Te}_2\text{O}_5$.³⁴⁴ All Li are in tetrahedral bonding environment.



LiAlTe_2

Material's Project ID	mp-4586
ICSD ID	280226
Space Group	$I\bar{4}2d$ [122]
Calculated Band Gap	2.6599 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	263.67 meV

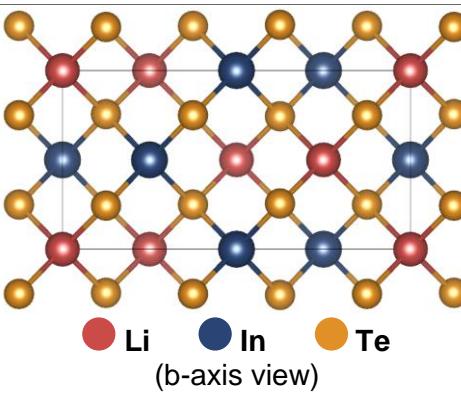
Notes: All Li are in a tetrahedral environment with corner sharing. The structure hasn't been examined as an ionic conductor – ongoing research is focused on optoelectronic properties.³⁴⁵



LiInTe_2

Material's Project ID	mp-20782
ICSD ID	658016
Space Group	$I\bar{4}2d$ [122]
Calculated Band Gap	1.7492 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	273.44 meV

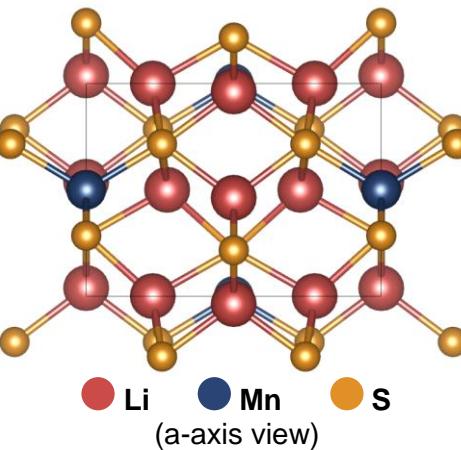
Notes: All Li are in a tetrahedral environment with corner sharing. The structure hasn't been examined as an ionic conductor – ongoing research is focused on optoelectronic properties.³⁴⁶



Li_6MnS_4

Material's Project ID	mp-756490
ICSD ID	NA
Space Group	$P4_2/nmc$ [137]
Calculated Band Gap	1.8508 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	273.44 meV

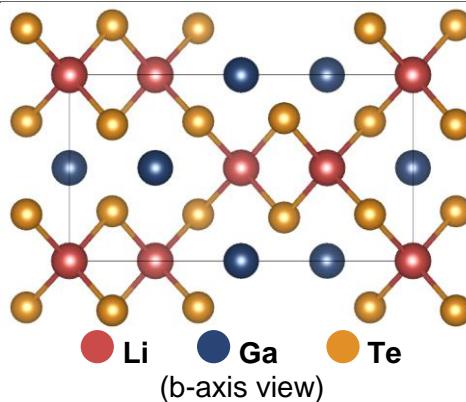
Notes: All Li are in an edge-sharing tetrahedral bonding environment. Augustine et al. posit that the structure could be a viable cathode material. They performed *ab-initio* calculations to measure the enthalpy of formation and have concluded that the structure should be stable.³⁴⁷



LiGaTe_2

Material's Project ID	mp-5048
ICSD ID	162555
Space Group	$I\bar{4}2d$ [122]
Calculated Band Gap	1.9666 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	273.44 meV

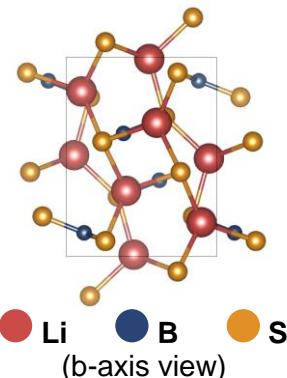
Notes: All Li are in a tetrahedral environment with corner sharing. The structure hasn't been examined as an ionic conductor – ongoing research is focused on optoelectronic properties.³⁴⁸ Isaenko et al. report an experimental band gap of 2.41 eV.



Li_3BS_3

Material's Project ID	mp-5614
ICSD ID	380104
Space Group	$Pnma$ [62]
Calculated Band Gap	3.0526 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	283.2 meV

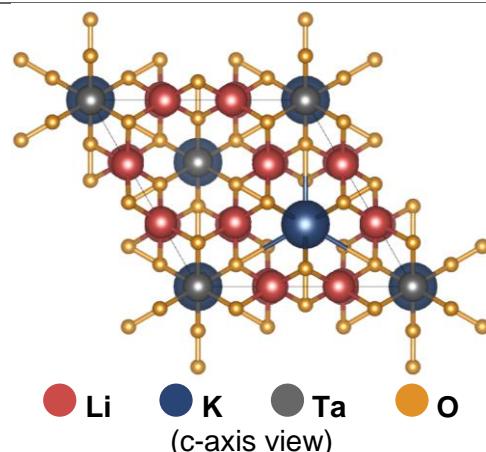
Notes: All Li are in a tetrahedral bonding environment. Recent NEB work suggests an activation barrier of 250 meV.³⁴⁹



KLi_6TaO_6

Material's Project ID	mp-9059
ICSD ID	73159
Space Group	$R\bar{3}mH$ [166]
Calculated Band Gap	4.4134 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	302.73 meV

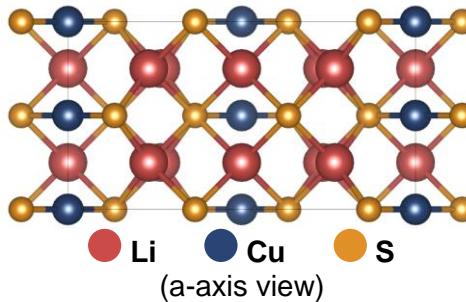
Notes: All Li are in a tetrahedral bonding environment with edge or corner sharing. Recent electrochemical characterization by Suzuki et al. found an ionic conductivity near 10^5 S cm^{-1} with aliovalent substitution of Sn.³⁵⁰



Li_3CuS_2

Material's Project ID	mp-1177695
ICSD ID	NA
Space Group	<i>Ibam</i> [72]
Calculated Band Gap	2.0826 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	312.5 meV

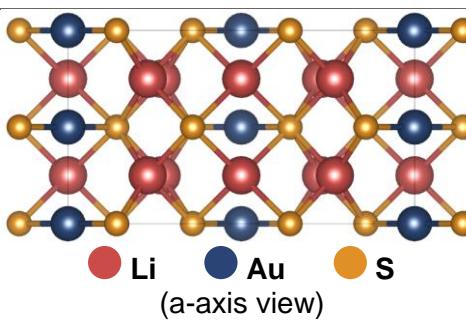
Notes: All Li are in an edge-sharing tetrahedral bonding environment. Explored for use as a cathode by Kawasaki et al. in 2021.³⁵¹ They found an initial charge-discharge capacity of 380 mAh g⁻¹ with average voltage of 2.1 V vs. Li/Li⁺.



Li_3AuS_2

Material's Project ID	mp-15999
ICSD ID	280535
Space Group	<i>Ibam</i> [72]
Calculated Band Gap	2.2827 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	312.5 meV

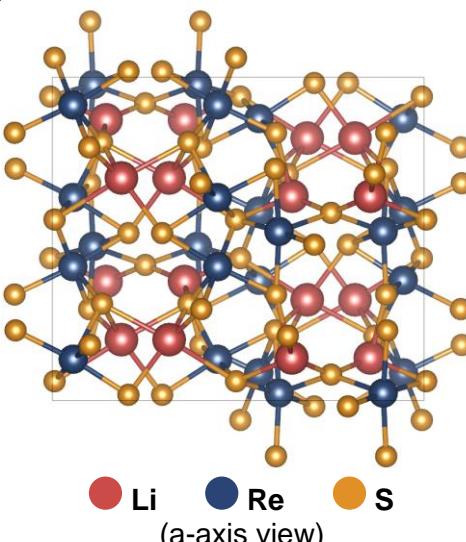
Notes: All Li are in an edge-sharing tetrahedral bonding environment. Never explored for battery purposes. Synthesis by Huang et al.³⁵²



$\text{Li}_4\text{Re}_6\text{S}_{11}$

Material's Project ID	mp-1181012
ICSD ID	NA
Space Group	<i>Pccn</i> [56]
Calculated Band Gap	1.7328 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	371.09 meV

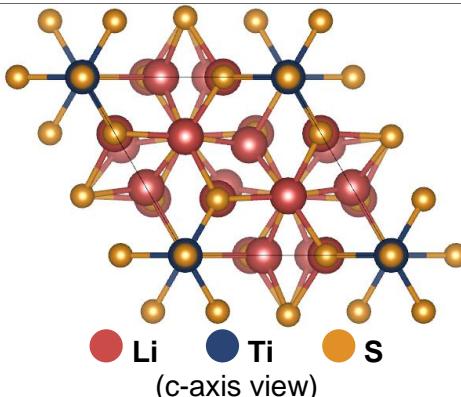
Notes: All Li sits in four- and five-coordinate environments. Kahle et al. previously screened ~1400 Li-containing compounds and identified $\text{Li}_4\text{Re}_6\text{S}_{11}$ as a potentially promising SSE using molecular dynamics simulation.³⁵³ Their simulations failed to resolve RT diffusion but found promising diffusivity at elevated temperatures.



Li₈TiS₆

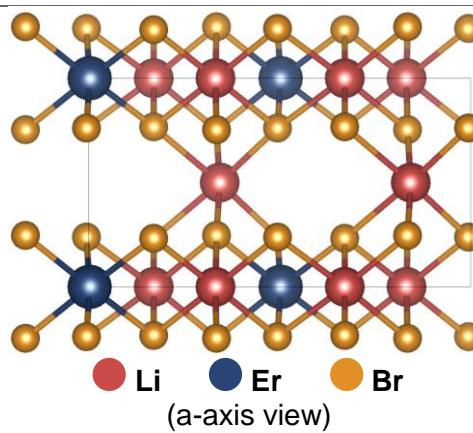
Material's Project ID	mp-753546
ICSD ID	NA
Space Group	$P6_3cm$ [185]
Calculated Band Gap	2.2925 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	380.86 meV

Notes: All Li are in a tetrahedral bonding environment.

**Li₃ErBr₆**

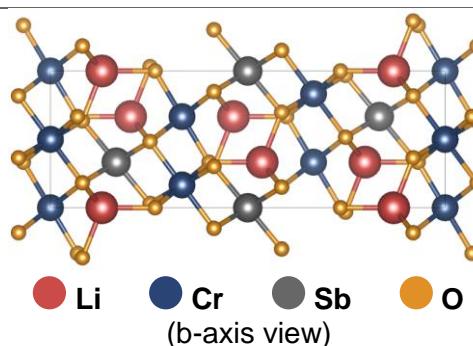
Material's Project ID	mp-1222492
ICSD ID	NA
Space Group	$C2$ [5]
Calculated Band Gap	4.4222 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	390.63 meV

Notes: All Li are in an octahedral bonding environment. Muy et al. identify Li₃ErBr₆ as one of eighteen promising compounds using a phonon-band descriptor approach.³⁵⁴ They synthesize the Cl analogue and report an experimental conductivity of 0.05-0.3 mS cm⁻¹. The material also mentioned briefly in perspective by Li et al.³⁵⁵

**Li₂Cr₃SbO₈**

Material's Project ID	mp-1178030
ICSD ID	NA
Space Group	$R\bar{3}m$ [166]
Calculated Band Gap	2.6513 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	419.92 meV

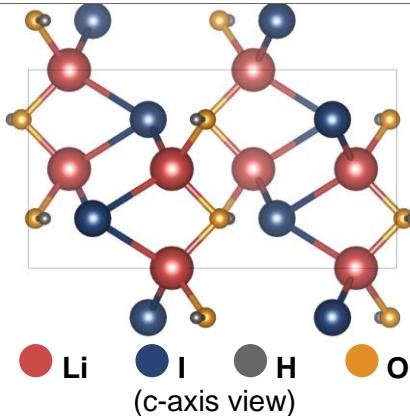
Notes: All Li are in a tetrahedral bonding environment.



Li_2HIO

Material's Project ID	mp-643069
ICSD ID	NA
Space Group	$Pnma$ [62]
Calculated Band Gap	4.3363 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	419.92 meV

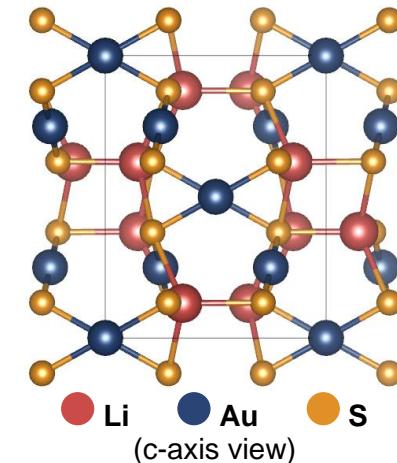
Notes: All Li are in a tetrahedral bonding environment. Sendek et al. identified Li_2HIO as promising using a combined ML and DFT approach.³⁵⁶ They predicted a RT diffusion barrier of 350 meV.



LiAuS

Material's Project ID	mp-29829
ICSD ID	165259
Space Group	$F22\bar{1}d$ [70]
Calculated Band Gap	1.587 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	439.45 meV

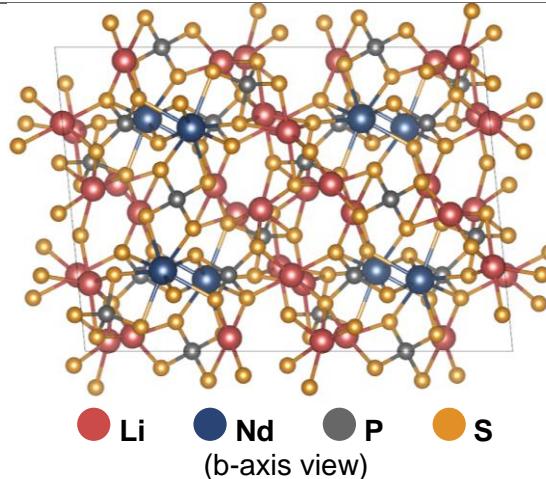
Notes: All Li are in an edge-sharing tetrahedral bonding environment. Synthesis via Huang et al.³⁵²



$\text{Li}_9\text{Nd}_2\text{P}_5\text{S}_{20}$

Material's Project ID	mp-1223032
ICSD ID	NA
Space Group	$C2/c$ [15]
Calculated Band Gap	2.6503 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	439.45 meV

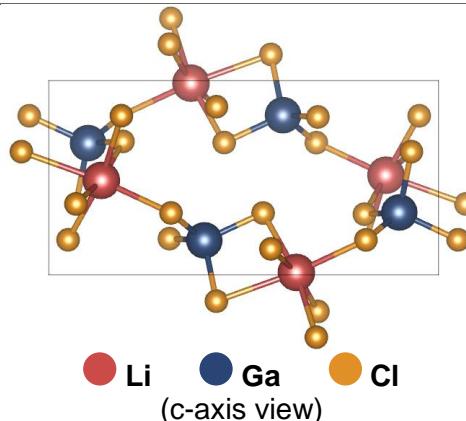
Notes: Li ions are in a distorted octahedral and some 5-coordinate bonding environments.



LiGaCl_4

Material's Project ID	mp-28341
ICSD ID	60849
Space Group	$P2_1/c$ [14]
Calculated Band Gap	4.4866 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	439.45 meV

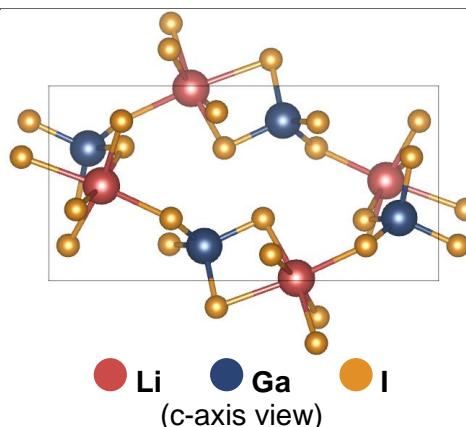
Notes: All Li are in an octahedral bonding environment. Mentioned briefly in perspective by Li et al.³⁵⁵



LiGal_4

Material's Project ID	mp-567967
ICSD ID	60850
Space Group	$P2_1/c$ [14]
Calculated Band Gap	2.4872 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	458.98 meV

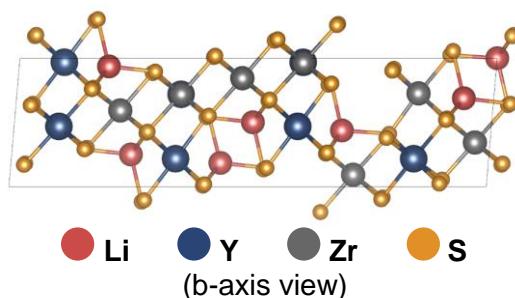
Notes: All Li are in an octahedral bonding environment. Discussed briefly in perspective by Li et al.³⁵⁵ Predicted by Kahle et al. to be a fast ionic conductor using molecular dynamics simulations.³⁵³ They predict an activation energy of 350 meV.



$\text{Li}_7\text{Y}_7\text{Zr}_9\text{S}_{32}$

Material's Project ID	mp-767467
ICSD ID	NA
Space Group	$P1$ [1]
Calculated Band Gap	1.0523 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	488.28 meV

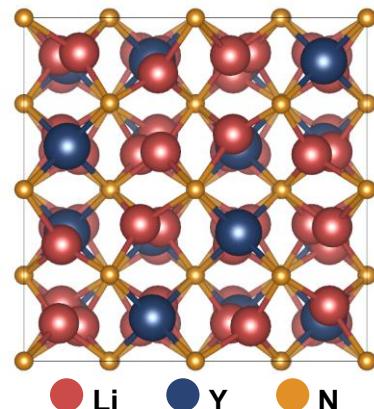
Notes: All Li are in a tetrahedral bonding environments.



Li₃YN₂

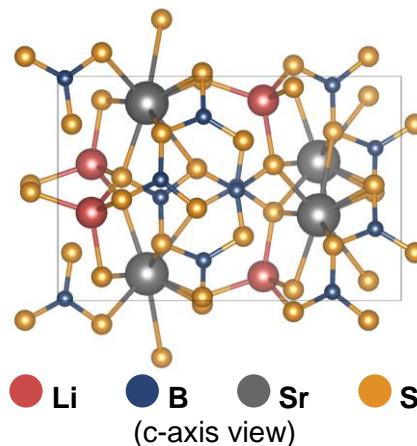
Material's Project ID	mp-1029592
ICSD ID	NA
Space Group	$Ia\bar{3}$ [206]
Calculated Band Gap	2.119 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	488.28 meV

Notes: All Li are in a three coordinate bonding environment.

**SrLiB₃S₆**

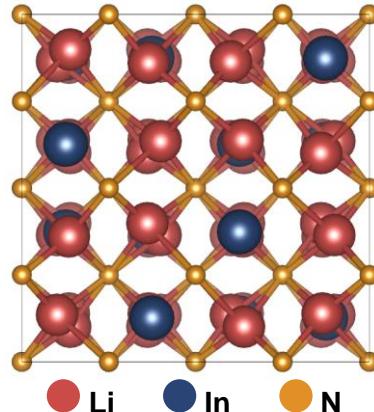
Material's Project ID	mp-558219
ICSD ID	79616
Space Group	Cc [9]
Calculated Band Gap	2.918 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	507.81 meV

Notes: All Li are in a tetrahedral bonding environment. Optical properties and air-stability have been briefly discussed by Kim et al.³⁵⁷

**Li₃InN₂**

Material's Project ID	mp-1029562
ICSD ID	NA
Space Group	$Ia\bar{3}$ [206]
Calculated Band Gap	1.0921 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	517.58 meV

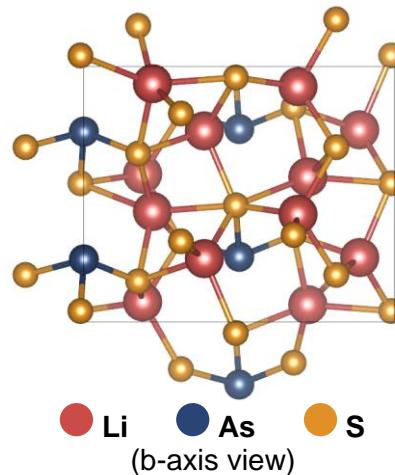
Notes: All Li are in an edge-sharing tetrahedral bonding environment. Synthetic accounts appear to exist in some books.



Li_3AsS_3

Material's Project ID	mp-28471
ICSD ID	424835
Space Group	$Pna2_1$ [33]
Calculated Band Gap	2.291 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	517.58 meV

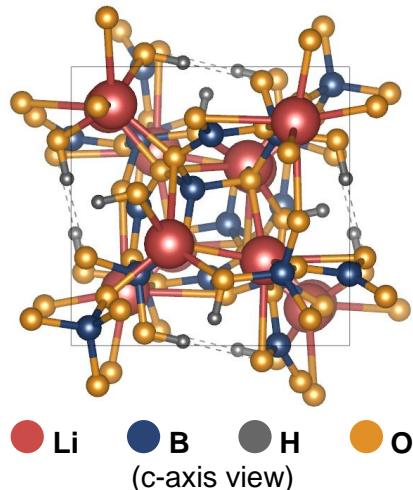
Notes: Li are all in an edge-sharing tetrahedral bonding environment. Wang et al. predicted that this might be a high-conductivity structure by using a “structure matching” algorithm.³⁵⁸



$\text{Li}_3\text{B}_5\text{H}_2\text{O}_8$

Material's Project ID	mp-1199091
ICSD ID	418166
Space Group	$P4_32_12$ [96]
Calculated Band Gap	5.8839 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	517.58 meV

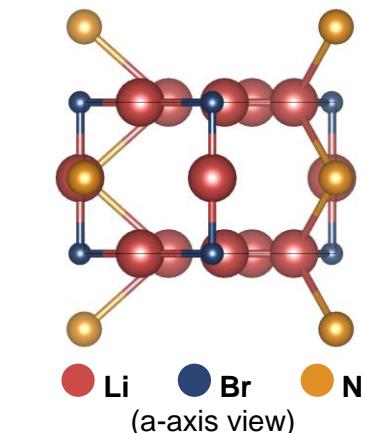
Notes: All Li are in a 5-coordinate bonding environment. A hydrothermal synthetic method has been described by Li et al.³⁵⁹



$\text{Li}_{10}\text{BrN}_3$

Material's Project ID	mp-28989
ICSD ID	78819
Space Group	$P\bar{6}m2$ [62]
Calculated Band Gap	1.4357 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	546.88 meV

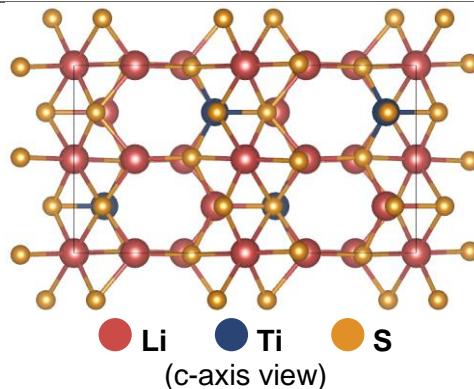
Notes: All Li are in 3-coordinate or 2-coordinate bonding environments. Identified by Snydacker et al. as a suitable coating for Li anode passivation via convex hull calculations.³⁶⁰



Li_4TiS_4

Material's Project ID	mp-766540
ICSD ID	NA
Space Group	$Pnma$ [62]
Calculated Band Gap	2.3811 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	546.88 meV

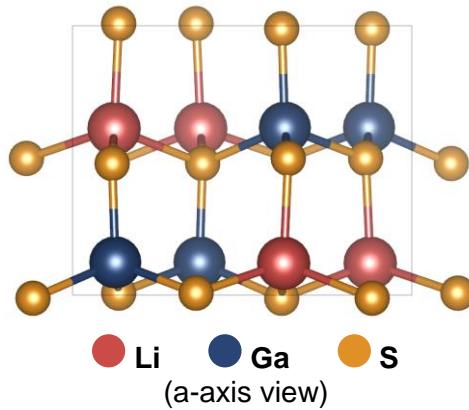
Notes: All Li are in octahedral or tetrahedral bonding environments. The tetrahedra sit between the octahedral layers. Amorphous Li_4TiS_4 is thought to form upon discharge of TiS_4 -based cathodes.³⁶¹



LiGaS_2

Material's Project ID	mp-3647
ICSD ID	68465
Space Group	$Pna2_1$ [33]
Calculated Band Gap	2.9659 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	546.88 meV

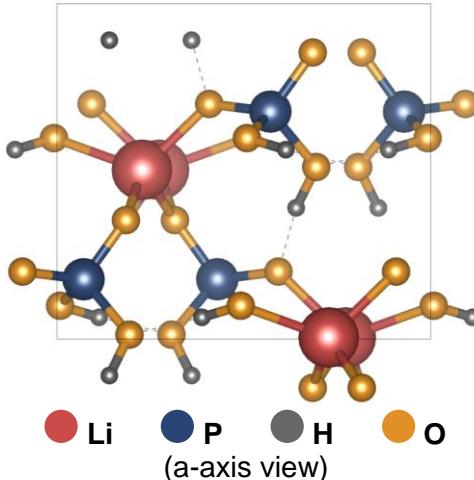
Notes: All Li are in a tetrahedral bonding environment. Wang et al. predicted that LiGaS_2 might be a high-conductivity structure by using a "structure matching" algorithm.³⁵⁸ Separately, He et al. used ab initio calculation to predict the same.³⁶²



LiPH_2O_4

Material's Project ID	mp-24610
ICSD ID	182308
Space Group	$Pna2_1$ [33]
Calculated Band Gap	5.5778 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	576.17 meV

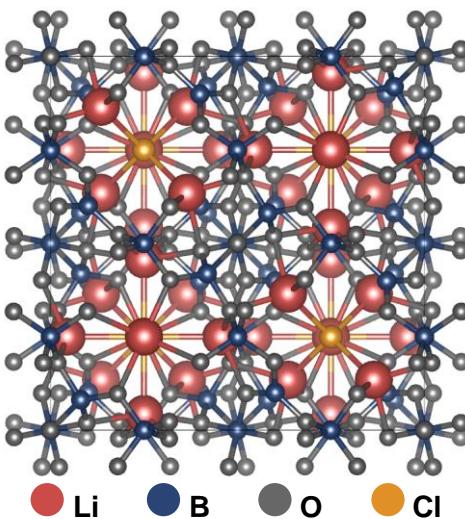
Notes: All Li are in a corner-sharing tetrahedral bonding environments.



$\text{Li}_{10}\text{B}_{14}\text{Cl}_2\text{O}_{25}$

Material's Project ID	mp-23122
ICSD ID	200981
Space Group	$F\bar{2}3$ [196]
Calculated Band Gap	6.3849 eV
Calculated E above E_{hull}	0 eV
Predicted Activation Energy	585.94 meV

Notes: Li are mostly in tetrahedral bonding environments, although some 5-coordinate environments exist. Kahle et al. identified $\text{Li}_{10}\text{B}_{14}\text{Cl}_2\text{O}_{25}$ as a potentially promising SSE material using a “pinball” model.³⁵³



b. Quasi-stable compounds (E_{hull} below 15 meV)

Excluding the labeled dataset, there are 34 compounds that are predicted to be within 15 meV of the convex hull (E_{hull}) and to exhibit a Li-hopping activation energy below 600 meV. Ten of the predicted compounds have already been experimentally examined and are hereafter excluded: Li_3SbS_4 , $\text{Li}_6\text{AsS}_5\text{I}$, $\text{Li}_6\text{PS}_5\text{I}$, Li_3ScCl_6 , Li_2MnBr_4 , Li_3N , $\text{LiTi}_2\text{P}_3\text{O}_{12}$, $\text{Li}_{10}\text{SiP}_2\text{S}_{12}$, Li_2ZnCl_4 , Li_3InO_3 . Another three are currently being excluded because they are used in cathodes: Li_3NbS_4 , Li_3CuS_2 , Li_6VCl_8 . The remaining 21 promising structures are discussed below and plotted by ascending activation energy in Figure S16.

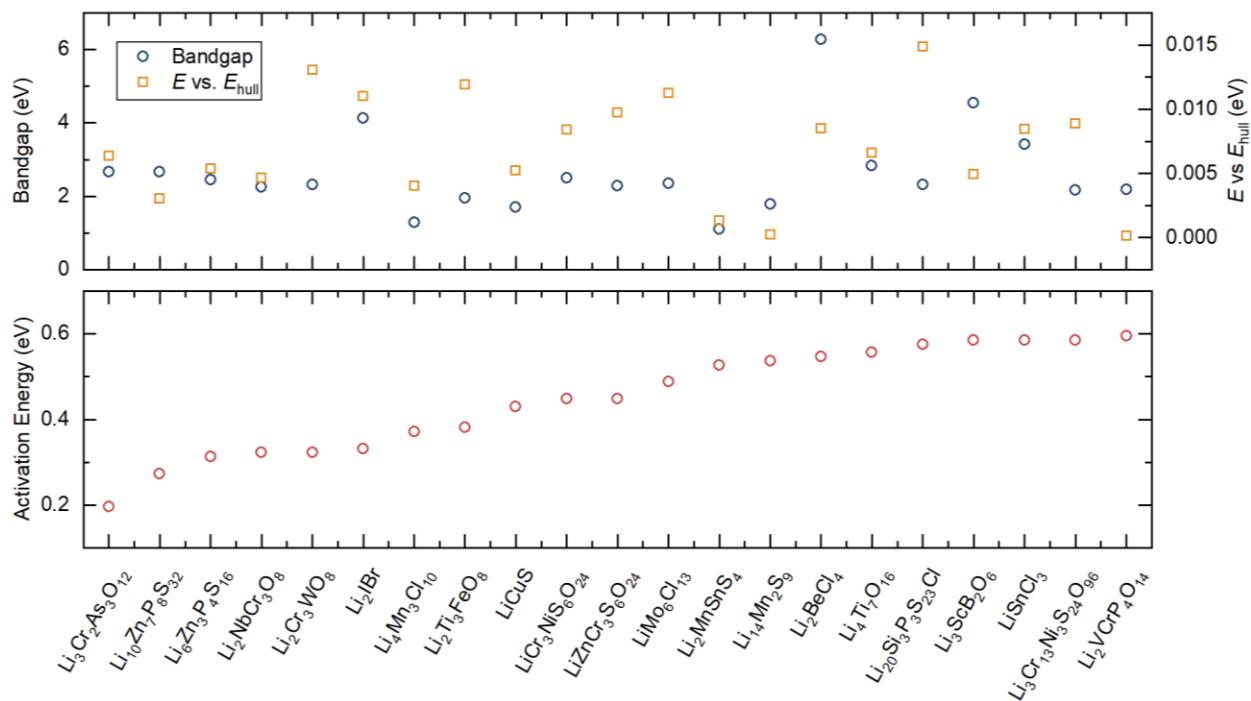
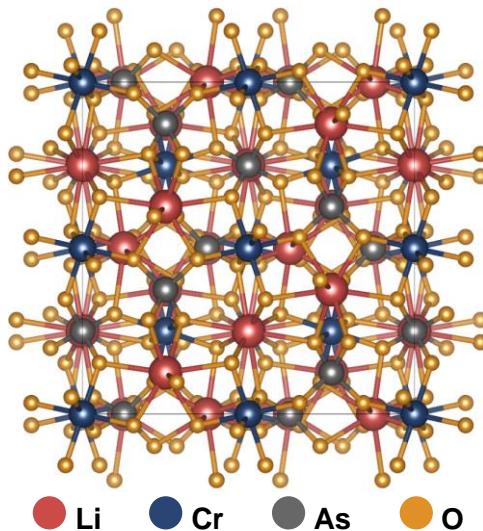


Figure S17. The 21 promising structures that are predicted to be within 15 meV of E_{hull} and to exhibit Li-hopping activation energy below 600 meV.

$\text{Li}_3\text{Cr}_2\text{As}_3\text{O}_{12}$

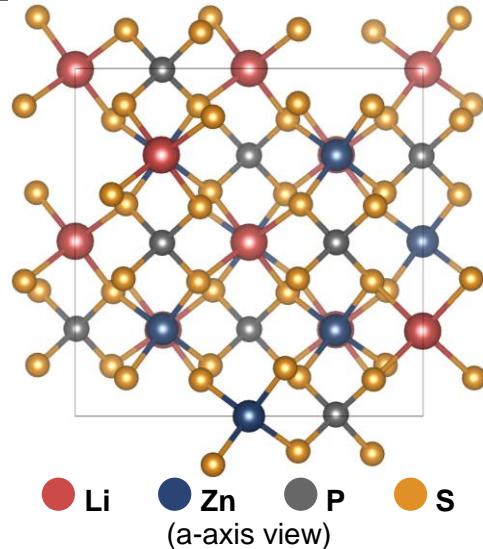
Material's Project ID	mp-779404
ICSD ID	NA
Space Group	$Ia\bar{3}d$ [230]
Calculated Band Gap	2.6702 eV
Calculated E above E_{hull}	6.37 meV
Predicted Activation Energy	165.31 meV

Notes: Li are in 8-coordinate sites surrounded by oxygens.

 **$\text{Li}_{10}\text{Zn}_7\text{P}_8\text{S}_{32}$**

Material's Project ID	mp-1147627
ICSD ID	NA
Space Group	$P1$ [1]
Calculated Band Gap	2.6635 eV
Calculated E above E_{hull}	3.04 meV
Predicted Activation Energy	273.44 meV

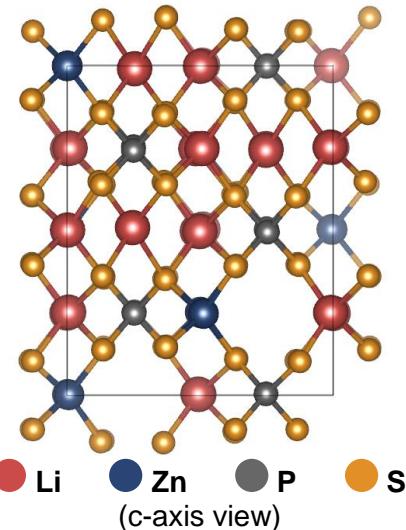
Notes: All Li are in tetrahedral bonding environments – corner sharing with Zn and P tetrahedra. Richard's et al. used NEB to predict that $\text{Li}_{10}\text{Zn}_7\text{P}_8\text{S}_{32}$ has a 252 meV activation energy for Li diffusion.³⁶³ They also predict a RT conductivity of 3.44 mS cm⁻¹.



$\text{Li}_6\text{Zn}_3\text{P}_4\text{S}_{16}$

Material's Project ID	mp-1147596
ICSD ID	NA
Space Group	$P\bar{1}$ [1]
Calculated Band Gap	2.4515 eV
Calculated E above E_{hull}	5.35 meV
Predicted Activation Energy	312.5 meV

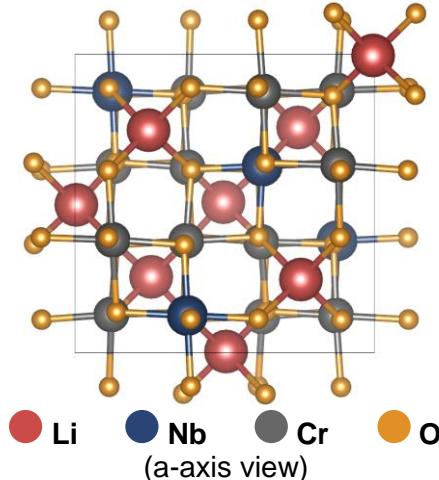
Notes: All Li are in tetrahedral bonding environments – corner sharing with Zn and P tetrahedra. Richard's et al. used NEB to predict that $\text{Li}_6\text{Zn}_3\text{P}_4\text{S}_{16}$ has a 181 meV activation energy for Li diffusion.³⁶³ They also predict a RT conductivity of 27.7 mS cm⁻¹.



$\text{Li}_2\text{NbCr}_3\text{O}_8$

Material's Project ID	mp-775164
ICSD ID	NA
Space Group	$P4_332$ [212]
Calculated Band Gap	2.2504 eV
Calculated E above E_{hull}	4.65 meV
Predicted Activation Energy	322.27 meV

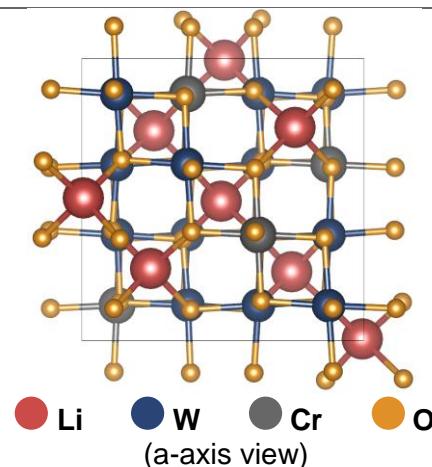
Notes: All Li are in tetrahedral bonding environments.



$\text{Li}_2\text{Cr}_3\text{WO}_8$

Material's Project ID	mp-758116
ICSD ID	NA
Space Group	$P4_332$ [212]
Calculated Band Gap	2.318 eV
Calculated E above E_{hull}	13.05 meV
Predicted Activation Energy	322.27 meV

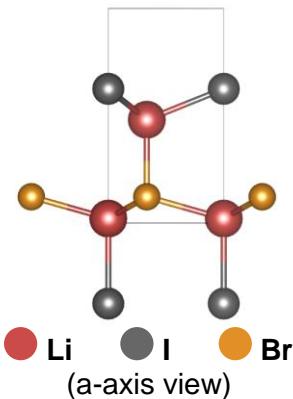
Notes: All Li are in tetrahedral bonding environments.



$\text{Li}_2\text{I}\text{Br}$

Material's Project ID	mp-1222669
ICSD ID	NA
Space Group	$P3m1$ [156]
Calculated Band Gap	4.1375 eV
Calculated E above E_{hull}	11.02 meV
Predicted Activation Energy	332.03 meV

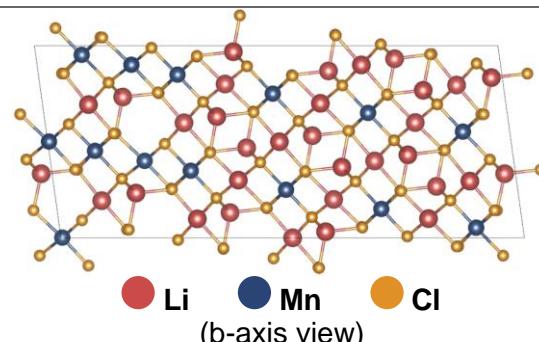
Notes: All Li are in tetrahedral bonding environment.



$\text{Li}_4\text{Mn}_3\text{Cl}_{10}$

Material's Project ID	mp-531376
ICSD ID	NA
Space Group	Cm [8]
Calculated Band Gap	1.2928 eV
Calculated E above E_{hull}	4.04 meV
Predicted Activation Energy	371.09 meV

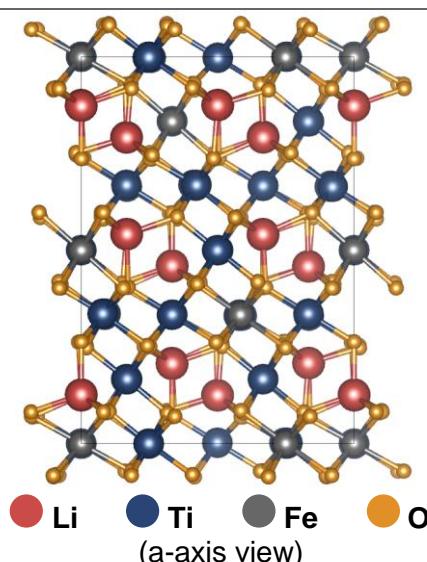
Notes: Octahedral Li layers with Li tetrahedra interspersed between.



$\text{Li}_2\text{Ti}_3\text{FeO}_8$

Material's Project ID	mp-775306
ICSD ID	NA
Space Group	$R\bar{3}2$ [155]
Calculated Band Gap	1.9461 eV
Calculated E above E_{hull}	11.9 meV
Predicted Activation Energy	380.86 meV

Notes: All Li are in tetrahedral bonding environments.



LiCuS

Material's Project ID mp-774736

ICSD ID NA

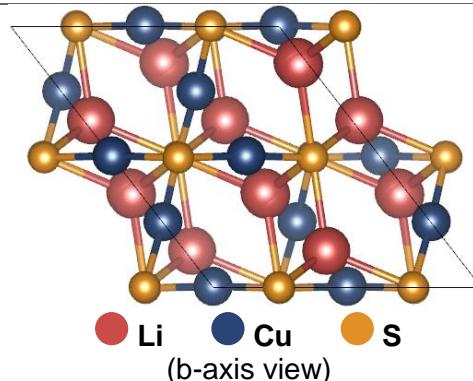
Space Group Cc [9]

Calculated Band Gap 1.6984 eV

Calculated E above E_{hull} 5.2 meV

Predicted Activation Energy 429.69 meV

Notes: All Li are in edge-sharing tetrahedral bonding environments. Previously examined as a cathode material by Chen et al.³⁶⁴



LiCr₃NiS₆O₂₄

Material's Project ID mp-766088

ICSD ID NA

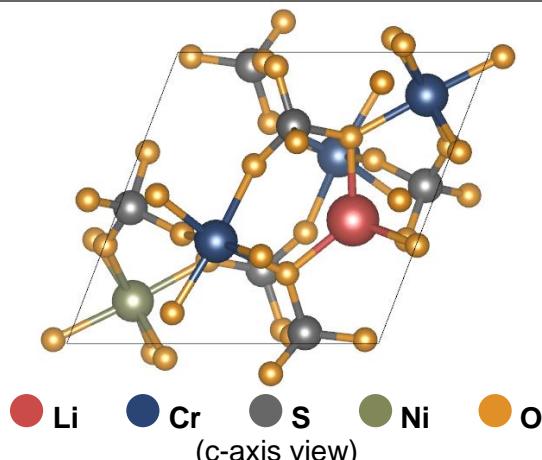
Space Group $P1$ [1]

Calculated Band Gap 2.5049 eV

Calculated E above E_{hull} 8.41 meV

Predicted Activation Energy 449.22 meV

Notes: All Li are in tetrahedral bonding environments.



LiZnCr₃S₆O₂₄

Material's Project ID mp-769549

ICSD ID NA

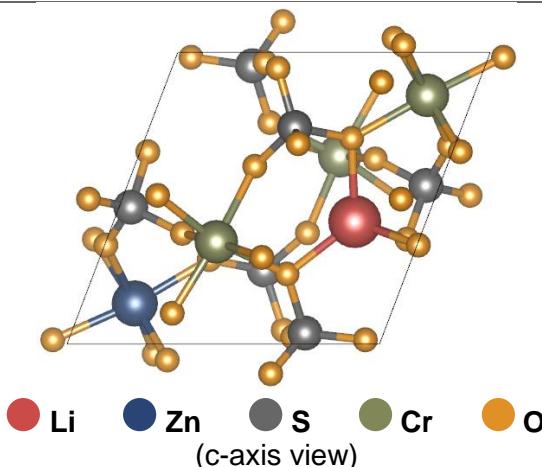
Space Group $P1$ [1]

Calculated Band Gap 2.2921 eV

Calculated E above E_{hull} 9.72 meV

Predicted Activation Energy 449.22 meV

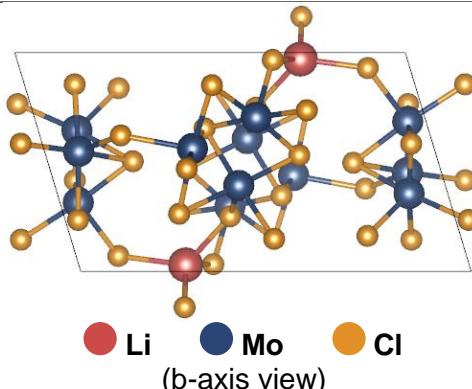
Notes: All Li are in tetrahedral bonding environments.



$\text{LiMo}_6\text{Cl}_{13}$

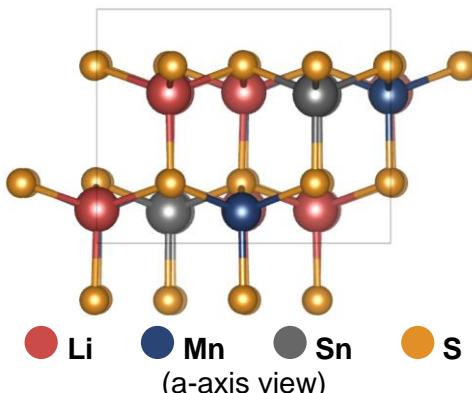
Material's Project ID	mp-680167
ICSD ID	410368
Space Group	$P\bar{1}$ [2]
Calculated Band Gap	2.3547 eV
Calculated E above E_{hull}	11.28 meV
Predicted Activation Energy	488.28 meV

Notes: All Li are in tetrahedral bonding environments.

 **$\text{Li}_2\text{MnSnS}_4$**

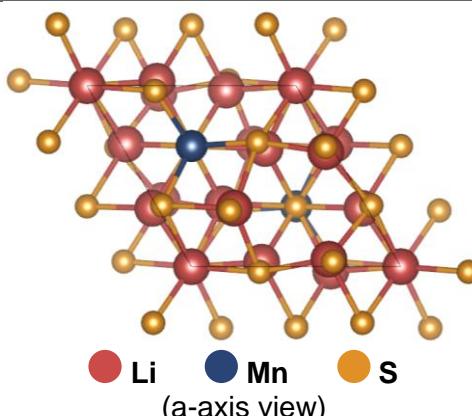
Material's Project ID	mp-1195603
ICSD ID	429817
Space Group	$Pna2_1$ [33]
Calculated Band Gap	1.1045 eV
Calculated E above E_{hull}	1.34 meV
Predicted Activation Energy	527.34 meV

Notes: All Li are in tetrahedral bonding environments. Devlin et al. have previously published a synthetic method for $\text{Li}_2\text{MnSnS}_4$.³⁶⁵

 **$\text{Li}_{14}\text{Mn}_2\text{S}_9$**

Material's Project ID	mp-756198
ICSD ID	NA
Space Group	$P\bar{3}$ [147]
Calculated Band Gap	1.7888 eV
Calculated E above E_{hull}	0.25 meV
Predicted Activation Energy	537.11 meV

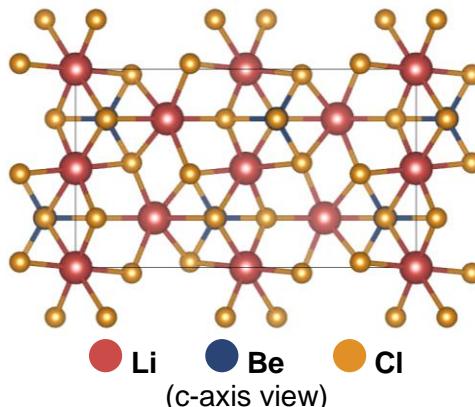
Notes: All Li are in edge-sharing tetrahedral bonding environments.



Li_2BeCl_4

Material's Project ID	mp-1210835
ICSD ID	NA
Space Group	$Pnma$ [62]
Calculated Band Gap	6.2881 eV
Calculated E above E_{hull}	8.52 meV
Predicted Activation Energy	546.88 meV

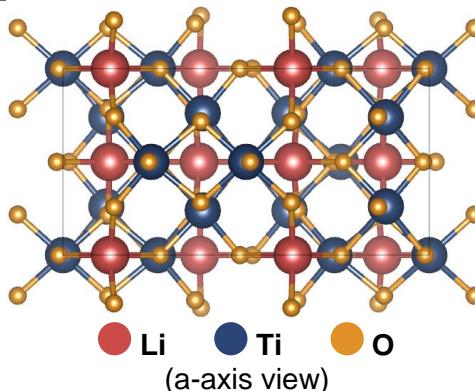
Notes: All Li are in edge-sharing octahedral bonding environments. A synthetic method has been published by Steiner et al.³⁶⁶



$\text{Li}_4\text{Ti}_7\text{O}_{16}$

Material's Project ID	mp-531820
ICSD ID	NA
Space Group	$Pnnm$ [58]
Calculated Band Gap	2.8323 eV
Calculated E above E_{hull}	6.62 meV
Predicted Activation Energy	556.64 meV

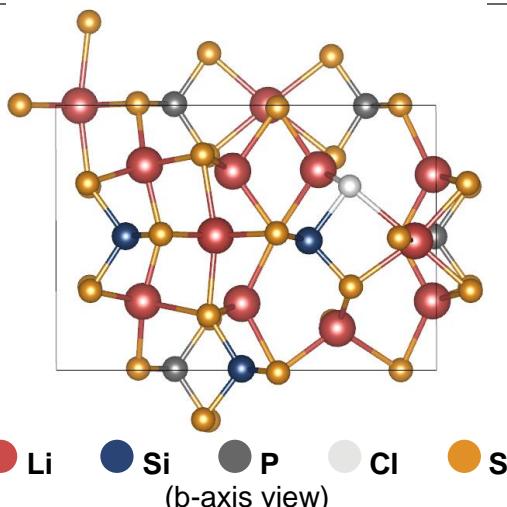
Notes: All Li are in tetrahedral bonding environments.



$\text{Li}_{20}\text{Si}_3\text{P}_3\text{S}_{23}\text{Cl}$

Material's Project ID	mp-1097035
ICSD ID	NA
Space Group	Pm [6]
Calculated Band Gap	2.3126 eV
Calculated E above E_{hull}	14.89 meV
Predicted Activation Energy	576.17 meV

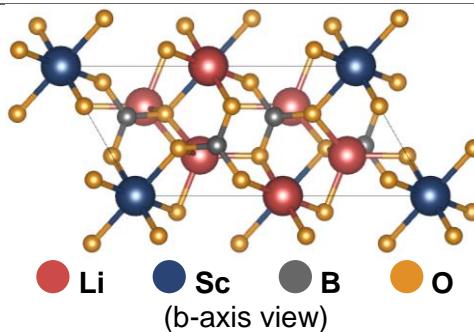
Notes: All Li are in corner-sharing tetrahedral bonding environments. $\text{Li}_{10}\text{Si}_3\text{P}_3\text{S}_{23}\text{Cl}$ was theoretically studied by Rao et al.³⁶⁷ They used it is a model system for a neural-network molecular dynamics pipeline.



$\text{Li}_3\text{ScB}_2\text{O}_6$

Material's Project ID	mp-557012
ICSD ID	241234
Space Group	$P2_1/c$ [14]
Calculated Band Gap	4.5457 eV
Calculated E above E_{hull}	4.93 meV
Predicted Activation Energy	585.94 meV

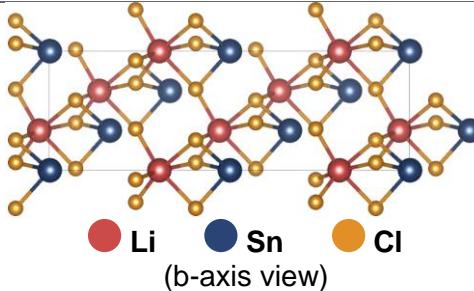
Notes: All Li are in tetrahedral or octahedral bonding environments.



LiSnCl_3

Material's Project ID	mp-998591
ICSD ID	NA
Space Group	$R3c$ [161]
Calculated Band Gap	3.4153 eV
Calculated E above E_{hull}	8.45 meV
Predicted Activation Energy	585.94 meV

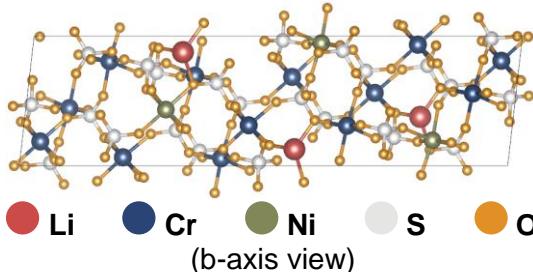
Notes: All Li are in octahedral bonding environments. Muy et al. examined LiSnCl_3 using a phonon-band descriptor approach.³⁵⁴ Despite a promising band-center value, they suggest it has a low stability window. Körbel et al. identify it as a promising piezoelectric material.³⁶⁸



$\text{Li}_3\text{Cr}_{13}\text{Ni}_3\text{S}_{24}\text{O}_{96}$

Material's Project ID	mp-695469
ICSD ID	NA
Space Group	$P1$ [1]
Calculated Band Gap	2.1679 eV
Calculated E above E_{hull}	8.9 meV
Predicted Activation Energy	585.94 meV

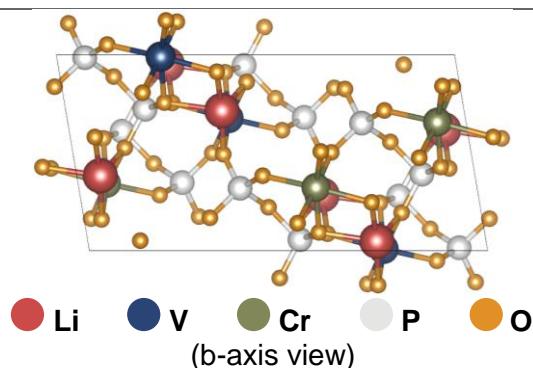
Notes: All Li are in tetrahedral bonding environments.



$\text{Li}_2\text{VCrP}_4\text{O}_{14}$

Material's Project ID	mp-759753
ICSD ID	NA
Space Group	$P1$ [1]
Calculated Band Gap	2.1798 eV
Calculated E above E_{hull}	0.13 meV
Predicted Activation Energy	595.7 meV

Notes: All Li are in distorted tetrahedral bonding environments.



c. Unknown-stability compounds (sans Materials Project entry)

There are 18 predictions that have no associated Material's Project entry. These structures lack stability data. Seven of the predicted compounds have already been experimentally examined and are hereafter excluded: Li_2O , Li_2S , $\text{Li}_7\text{Y}_7\text{Zr}_9\text{S}_{32}$, $\text{Li}_4\text{SnSe}_4\text{O}_{13}$, Li_2MnBr_4 , Li_5AlS_4 , $\text{Li}_3\text{Fe}_2\text{P}_3\text{O}_{12}$. Another five are currently being excluded because they are used in cathodes: $\text{Li}_2\text{Mn}_3\text{NiO}_8$, $\text{Li}_2\text{Mn}_3\text{CoO}_8$, $\text{Li}_5\text{Mn}_{16}\text{O}_{32}$, $\text{Li}_2\text{Mn}_{15}\text{AlO}_{32}$, $\text{Li}_3\text{V}_2\text{P}_3\text{O}_{12}$. The remaining 6 promising structures are discussed below and plotted in order of ascending activation energy in Figure S17.

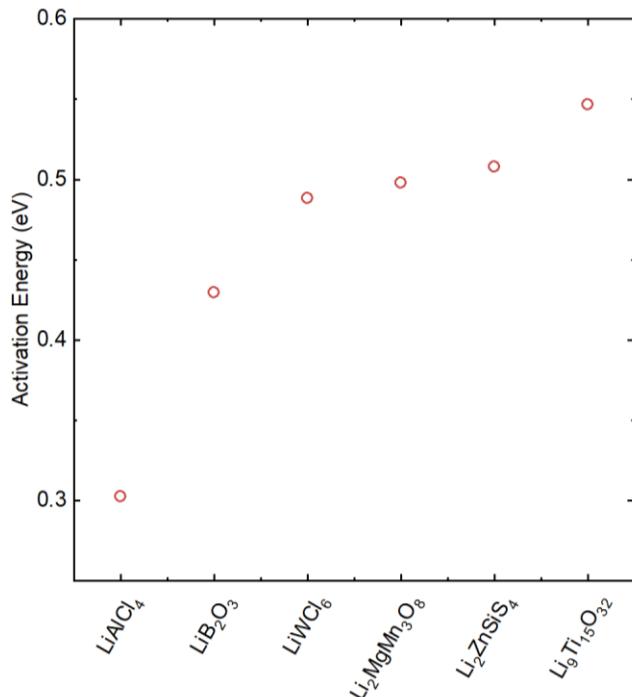
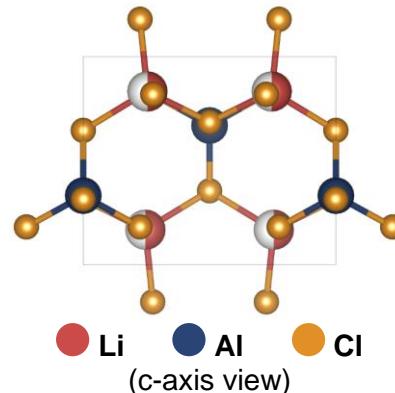


Figure S18. The six promising structures that lack Materials Project data but are predicted to exhibit Li-hopping activation energy below 600 meV.

LiAlCl_4

Material's Project ID	NA
ICSD ID	244127
Space Group	$Pmn2_1$ [31]
Calculated Band Gap	NA
Calculated E above E_{hull}	NA
Predicted Activation Energy	302.73 meV

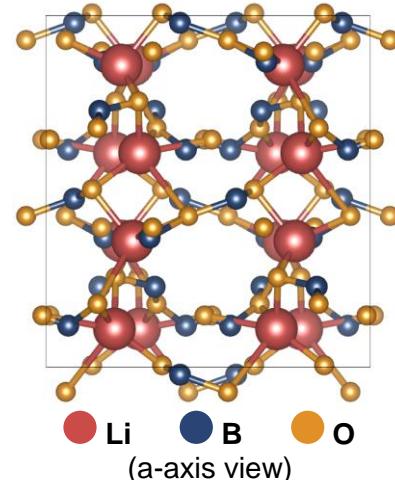
Notes: All Li are in tetrahedral bonding environments. Synthetic method by Prömper et al.³⁶⁹



LiB_2O_3

Material's Project ID	NA
ICSD ID	183930
Space Group	$I4_1cd$ [110]
Calculated Band Gap	NA
Calculated E above E_{hull}	NA
Predicted Activation Energy	429.69 meV

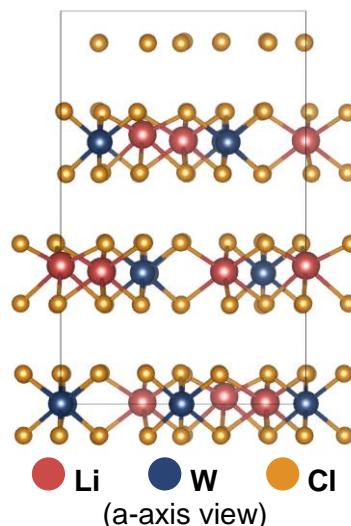
Notes: All Li are in 5-coordinate bonding environments. Previously studied by Abdel-Khalek et al. in a glass ceramic.³⁷⁰ Discussed in some detail by Rousse et al.³⁷¹



LiWCl_6

Material's Project ID	NA
ICSD ID	409938
Space Group	$R\bar{3}H$ [146]
Calculated Band Gap	NA
Calculated E above E_{hull}	NA
Predicted Activation Energy	488.28 meV

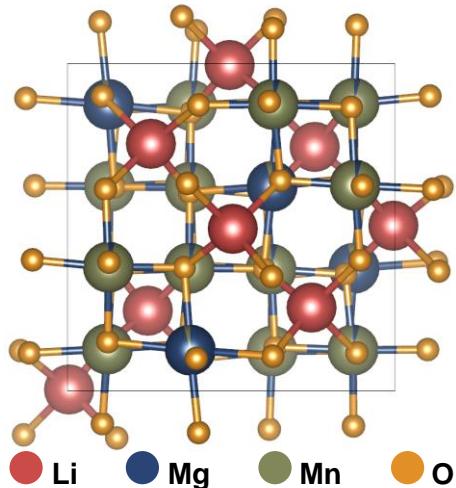
Notes: All Li are in octahedral bonding environments.



Li₂MgMn₃O₈

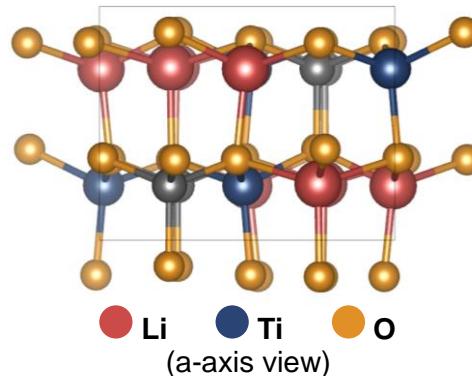
Material's Project ID	NA
ICSD ID	94758
Space Group	$P4_332$ [212]
Calculated Band Gap	NA
Calculated E above E_{hull}	NA
Predicted Activation Energy	498.05 meV

Notes: All Li are in tetrahedral bonding environments. Synthetic method by Branford et al.³⁷²

**Li₂ZnSiS₄**

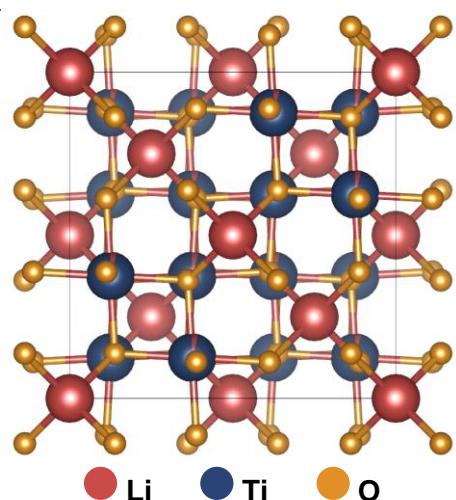
Material's Project ID	NA
ICSD ID	264457
Space Group	$Pna2_1$ [33]
Calculated Band Gap	NA
Calculated E above E_{hull}	NA
Predicted Activation Energy	507.81 meV

Notes: All Li are in tetrahedral bonding environments. A melt flux synthesis has been developed by Li et al – they examined the material for second-harmonic generation response.³⁷³

**Li₉Ti₁₅O₃₂**

Material's Project ID	NA
ICSD ID	15790
Space Group	$Fd\bar{3}mS$ [227]
Calculated Band Gap	NA
Calculated E above E_{hull}	NA
Predicted Activation Energy	546.88 meV

Notes: Most Li are in tetrahedral bonding environments, with some partial substitution onto the octahedral Ti sites.



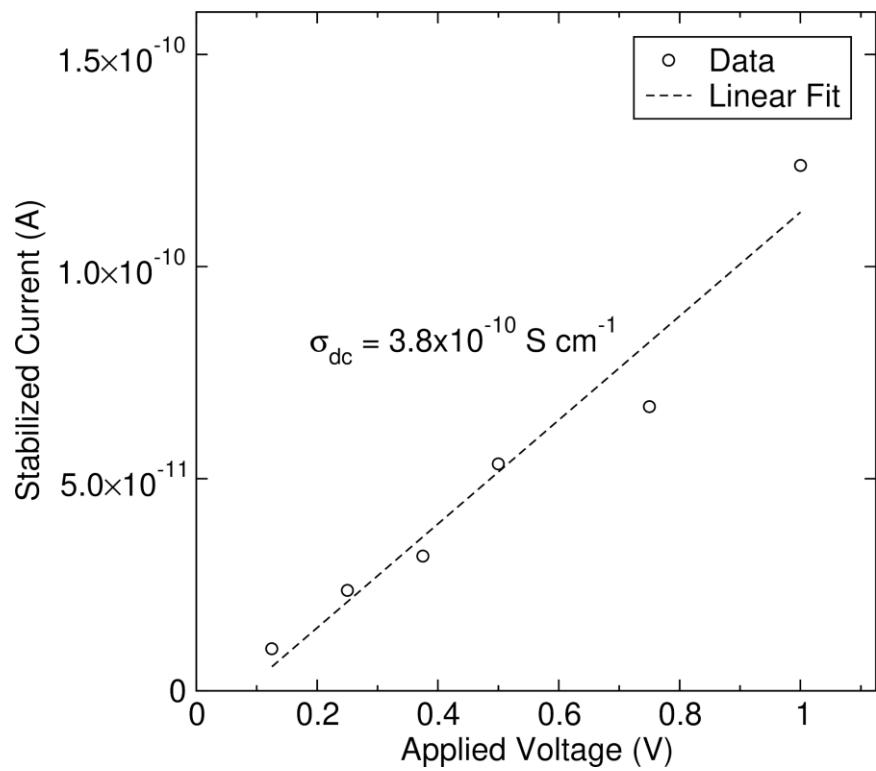


Figure S19. Steady-state current of Au/a-Li_{2.95}B_{0.95}Si_{0.05}S₃/Au cell for different voltage polarizations.
Measurements were done at 25°C with applied voltages of 0.125 V, 0.25 V, 0.375 V, 0.5 V and 1.0 V.

Citations:

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